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SECTION: 3.1.1.1.1.1.1

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## BRIEF DESCRIPTION:

THIS SECTION CONTAINS SIX PROCEDURES:  
DEC PERFORMS A TRIANGULAR DECOMPOSITION WITH PARTIAL PIVOTING;  
GSSELM PERFORMS A TRIANGULAR DECOMPOSITION WITH A COMBINATION OF  
PARTIAL AND COMPLETE PIVOTING;  
QENRMINV DELIVERS THE 1-NORM OF THE INVERSE OF A MATRIX WHOSE  
TRIANGULARLY DECOMPOSED FORM IS DELIVERD BY DEC OR GSSELM;  
ERBELM CALCULATES A ROUGH UPPERBOUND FOR THE SOLUTION OF A LINEAR  
SYSTEM WHOSE MATRIX IS TRIANGULARLY DECOMPOSED BY GSSELM;  
GSSERB PERFORMS A TRIANGULAR DECOMPOSTION OF THE MATRIX OF A LINEAR  
SYSTEM AND CALCULATES AN UPPERBOUND FOR THE RELATIVE ERROR OF THE  
SOLUTION OF THAT SYSTEM;  
GSSNRI PERFORMS A TRIANGULAR DECOMPOSITION AND CALCULATES THE  
1-NORM OF THE INVERSE MATRIX;

THE METHOD USED IN DEC AND GSSELM YIELDS A LOWER-TRIANGULAR MATRIX  
L AND A UNIT UPPER-TRIANGULAR MATRIX U SUCH THAT THE PRODUCT  
LU EQUALS THE GIVEN MATRIX WITH PERMUTED ROWS (DEC) OR ROWS AND  
COLUMNS (GSSELM); IN DEC, ONLY PARTIAL PIVOTING IS USED ([3],  
[4, P.115], [5, P.201]); THE PIVOTING STRATEGY IN GSSELM IS  
A COMBINATION OF PARTIAL AND COMPLETE PIVOTING ([2], [1]); IN THIS  
STRATEGY THE PROCESS WILL SWITCH TO COMPLETE PIVOTING IF PARTIAL  
PIVOTING MIGHT NOT YIELD STABLE RESULTS; SO IN GSSELM THE  
EFFICIENCY OF PARTIAL PIVOTING IS COMBINED WITH THE STABILITY OF  
COMPLETE PIVOTING;  
SINCE, IN EXCEPTIONAL CASES, PARTIAL PIVOTING MAY YIELD USELESS  
RESULTS, EVEN FOR WELL-CONDITIONED MATRICES, THE USER IS ADVISED TO  
USE GSSELM; HOWEVER, IF THE NUMBER OF VARIABLES IS SMALL RELATIVE  
TO THE NUMBER OF BINARY DIGITS IN THE NUMBER REPRESENTATION, THEN  
DEC MAY ALSO BE USED;

## KEYWORDS:

LU DECOMPOSITION,  
TRIANGULAR DECOMPOSITION,  
GAUSSIAN ELIMINATION.

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SUBSECTION: DEC.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:

"PROCEDURE" DEC(A, N, AUX, P); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX; "INTEGER" "ARRAY" P;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE MATRIX;  
 EXIT: THE CALCULATED LOWER-TRIANGULAR MATRIX AND UNIT  
 UPPERTRIANGULAR MATRIX WITH ITS UNIT DIAGONAL OMITTED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[1:3];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;

EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R  
 IS POSITIVE, ELSE AUX[1] = -1;

AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 AUX[3] < N THEN THE PROCESS IS BROKEN OFF, BECAUSE  
 THE SELECTED PIVOT IS TOO SMALL RELATIVE TO A  
 MATRIX NORM;

P: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" P[1:N];  
 EXIT: THE PIVOTAL INDICES.

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PROCEDURES USED:

MATMAT = CP34013,  
 MATTAM = CP34015,  
 ICHROW = CP34032.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: DEC DECLARES A ONE-DIMENSIONAL AUXILIARY REAL ARRAY OF ORDER N.

RUNNING TIME: PROPORTIONAL TO  $N^{**}3$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE TRIANGULAR DECOMPOSITION IS PERFORMED IN AT MOST N STEPS; THE K-TH STEP,  $K=1, \dots, N$ , PRODUCES THE K-TH COLUMN OF THE LOWER-TRIANGULAR MATRIX L; SUBSEQUENTLY, THE PIVOT IS SELECTED IN THIS COLUMN; IF THIS PIVOT IS LESS THAN AUX(2) TIMES THE MAXIMUM OF THE EUCLIDIAN NORMS OF THE ROWS, THEN THE PROCESS IS BROKEN OFF, ELSE THE PIVOTAL ROW AND THE K-TH ROW OF THE MATRIX ARE INTERCHANGED; FINALLY THE K-TH ROW OF THE UNIT UPPER-TRIANGULAR MATRIX U IS PRODUCED; THAT ELEMENT OF THE K-TH COLUMN OF L IS CHOSEN AS PIVOT, WHOSE ABSOLUTE VALUE DIVIDED BY THE EUCLIDIAN NORM OF THE CORRESPONDING ROW OF THE MATRIX, IS MAXIMAL; THUS, THE MATRIX IS EQUILIBRATED IN THIS PIVOTING STRATEGY, SUCH THAT THE ROWS EFFECTIVELY OBTAIN UNIT EUCLIDIAN NORM.

EXAMPLE OF USE: SEE DECSOL (SECTION 3.1.1.1.1.1.3).

SUBSECTION: GSSELM .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" GSSELM(A, N, AUX, RI, CI); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX; "INTEGER" "ARRAY" RI, CI;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE N-TH ORDER MATRIX;  
 EXIT: THE CALCULATED LOWER-TRIANGULAR MATRIX AND UNIT  
 UPPERTRIANGULAR MATRIX WITH ITS UNIT DIAGONAL OMITTED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[1:7];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 AUX[4]: A VALUE WHICH IS USED FOR CONTROLLING PIVOTING;  
 USUALLY, AUX[4] = 8 WILL GIVE GOOD RESULTS;

EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R  
 IS POSITIVE, ELSE AUX[1] = -1;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 AUX[3] < N THEN THE PROCESS IS BROKEN OFF, BECAUSE  
 THE SELECTED PIVOT IS TOO SMALL RELATIVE TO A  
 MATRIX NORM;  
 AUX[5]: THE MODULUS OF AN ELEMENT WHICH IS OF MAXIMUM  
 ABSOLUTE VALUE FOR THE MATRIX GIVEN IN ARRAY A;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH (I. E. THE MODULUS OF  
 AN ELEMENT WHICH IS OF MAXIMUM ABSOLUTE VALUE FOR  
 THE MATRICES OCCURRING DURING ELIMINATION);

RI: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" RI[1:N];  
 EXIT: THE PIVOTAL ROW-INDICES;

CI: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" CI[1:N];  
 EXIT: THE PIVOTAL COLUMN INDICES;

## PROCEDURES USED:

ROWCST	=	CP31132,
ELMROW	=	CP34024,
MAXELMROW	=	CP34025,
ICHCOL	=	CP34031,
ICHROW	=	CP34032,
MAXMAT	=	CP34230.

RUNNING TIME: PROPORTIONAL TO  $N^{**}3$ .

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

THE PROCESS OF GAUSSIAN ELIMINATION IS PERFORMED IN AT MOST  $N$  STEPS, WHERE  $N$  DENOTES THE ORDER OF THE MATRIX; PARTIAL PIVOTING WILL BE USED AS LONG AS THE CALCULATED UPPER BOUND FOR THE GROWTH ([2], [1]), IS LESS THAN A CRITICAL VALUE THAT EQUALS  $AUX[2] * N$  TIMES THE MODULUS OF AN ELEMENT WHICH IS OF MAXIMUM ABSOLUTE VALUE FOR THE GIVEN MATRIX; IN THE PARTIAL PIVOTING STRATEGY, THAT ELEMENT IS CHOSEN AS PIVOT IN THE  $K$ -TH STEP, WHOSE ABSOLUTE VALUE IS MAXIMAL FOR THE  $K$ -TH COLUMN OF THE LOWER-TRIANGULAR MATRIX  $L$ ; HOWEVER, IF THE UPPER BOUND FOR THE GROWTH EXCEEDS THIS CRITICAL VALUE IN THE  $K$ -TH STEP, THEN A PIVOT IS SELECTED IN THE  $J$ -TH STEP ( $J = K, \dots, N$ ), IN SUCH A WAY, THAT ITS ABSOLUTE VALUE IS MAXIMAL FOR THE REMAINING SUBMATRIX OF ORDER  $N - K + 1$  (COMPLETE PIVOTING); SINCE IN PRACTICE, IF WE CHOOSE  $AUX[4]$  PROPERLY, THE UPPER BOUND FOR THE GROWTH RARELY EXCEEDS THIS CRITICAL VALUE ([2], [4]), WE WILL USUALLY TAKE ADVANTAGE OF THE GREATER SPEED OF PARTIAL PIVOTING (ORDER  $N - K + 1$  IN THE  $K$ -TH STEP), WHILE IN A FEW DOUBTFUL CASES NUMERICAL DIFFICULTIES WILL BE RECOGNIZED AND THE PROCESS WILL SWITCH TO COMPLETE PIVOTING (ORDER  $(N - K + 1) ** 2$  IN THE  $K$ -TH STEP); USING GSSELM, THE UPPER BOUND FOR THE RELATIVE ERROR IN THE SOLUTION OF A LINEAR SYSTEM ([4], [5]), WILL BE AT MOST  $AUX[4] * N$  TIMES THE UPPER BOUND USING GAUSSIAN ELIMINATION WITH COMPLETE PIVOTING ONLY; USUALLY, HOWEVER, THIS WILL BE A CRUDE OVERESTIMATE; THE CHOICE  $AUX[4] < 1 / N$  WILL RESULT IN COMPLETE PIVOTING ONLY, WHILE PARTIAL PIVOTING WILL BE USED IN EVERY STEP IF WE CHOOSE  $AUX[4] > 2 * (N - 1) / N$ ; USUALLY,  $AUX[4] = 8$  WILL GIVE GOOD RESULTS ([2], [1]);

THE PROCESS WILL ALSO SWITCH TO COMPLETE PIVOTING IF THE MODULUS OF THE PIVOT OBTAINED WITH PARTIAL PIVOTING IS LESS THAN A CERTAIN TOLERANCE, WHICH EQUALS THE GIVEN RELATIVE TOLERANCE  $AUX[2]$  TIMES THE MODULUS OF AN ELEMENT WHICH IS OF MAXIMUM ABSOLUTE VALUE FOR THE GIVEN MATRIX; IF ALL ELEMENTS IN THE REMAINING SUBMATRIX ARE SMALLER IN ABSOLUTE VALUE THAN THIS TOLERANCE THEN THE PROCESS IS BROKEN OFF AND THE PREVIOUS STEPNUMBER IS DELIVERED IN  $AUX[3]$ ; IN CONTRAST WITH THE METHOD USED IN DEC (THIS SECTION), NO EQUILIBRATING IS DONE IN THIS PIVOTING STRATEGY; THE USER HIMSELF HAS TO TAKE CARE FOR A REASONABLE SCALING OF THE MATRIX ELEMENTS,

EXAMPLE OF USE: SEE GSSSQL (SECTION 3.1.1.1.1.1.3).

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SUBSECTION: ONENRMINV.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS  
 "REAL" "PROCEDURE" ONENRMINV(A, N); "VALUE" N;  
 "INTEGER" N; "ARRAY" A;

ONENRMINV:= THE 1-NORM OF THE CALCULATED INVERSE OF THE MATRIX,  
 WHOSE TRIANGULARLY DECOMPOSED FORM IS GIVEN IN ARRAY A;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];

ENTRY:

THE TRIANGULARLY DECOMPOSED FORM OF A MATRIX, AS DELIVERED  
 BY GSSELM OR DEC (THIS SECTION);

N: <ARITHMETICAL EXPRESSION>;

THE ORDER OF THE MATRIX, WHOSE TRIANGULARLY DECOMPOSED  
 FORM IS GIVEN IN ARRAY A.

PROCEDURES USED:

MATVEC = CP34011.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: ONENRMINV DECLARES A ONE-DIMENSIONAL  
 AUXILIARY REAL ARRAY OF ORDER N.

RUNNING TIME: PROPORTIONAL TO  $N^{**}3$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE INVERSE OF THE MATRIX WHOSE TRIANGULARLY DECOMPOSED FORM, AS  
 DELIVERED BY GSSELM OR DEC, IS GIVEN IN ARRAY A, IS CALCULATED WITH  
 FORWARD AND BACK SUBSTITUTION ([3], [4], [5]); ONLY THE 1-NORM OF  
 THIS INVERSE IS DELIVERED BY ONENRMINV; THE ELEMENTS OF ARRAY A  
 REMAIN UNALTERED.

EXAMPLE OF USE: SEE GSSSOLERB (SECTION 3.1.1.1.1.1.3).

SUBSECTION: ERBELM.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" ERBELM(N, AUX, NRMINV); "VALUE" N, NRMINV;  
 "INTEGER" N; "REAL" NRMINV; "ARRAY" AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETICAL EXPRESSION>;  
 THE ORDER OF THE LINEAR SYSTEM IN CONSIDERATION;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[0:11];

ENTRY:

AUX[0]: THE MACHINE PRECISION;

AUX[5]: THE MODULUS OF AN ELEMENT, WHICH IS OF MAXIMUM  
 ABSOLUTE VALUE FOR THE MATRIX OF THE LINEAR SYSTEM;  
 THIS VALUE IS DELIVERED BY GSSELM IN AUX[5] (THIS  
 SECTION);

AUX[6]: AN UPPER BOUND FOR THE RELATIVE ERROR IN THE  
 ELEMENTS OF THE MATRIX OF THE LINEAR SYSTEM;

AUX[7]: AN UPPER BOUND FOR THE GROWTH DURING GAUSSIAN  
 ELIMINATION; THIS VALUE IS DELIVERED IN AUX[7] BY  
 GSSELM (THIS SECTION);

EXIT:

AUX[9]: THE VALUE OF NRMINV;

AUX[11]: A ROUGH UPPER BOUND FOR THE RELATIVE ERROR IN THE  
 SOLUTION OF A LINEAR SYSTEM WHEN GAUSSIAN  
 ELIMINATION IS USED FOR THE CALCULATION OF THIS  
 SOLUTION; IF NO USE CAN BE MADE OF THE FORMULA FOR  
 THE ERROR BOUND (SEE: METHOD AND PERFORMANCE),  
 BECAUSE OF A VERY BAD CONDITION OF THE MATRIX, THEN  
 AUX[11]:= -1;

NRMINV: <ARITHMETICAL EXPRESSION>;  
 THE 1-NORM OF THE INVERSE OF THE MATRIX OF THE LINEAR  
 SYSTEM MUST BE GIVEN IN NRMINV.



SECTION: 3.1.1.1.1.1.1

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PROCEDURES USED: NONF.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

WHEN CALLED AFTER GSSELM, ERBELM WILL CALCULATE A ROUGH UPPER BOUND FOR THE RELATIVE ERROR IN THE SOLUTION OF THE LINEAR SYSTEM, WHOSE MATRIX IS DECOMPOSED INTO TRIANGULAR FORM BY GSSELM (THIS SECTION); THE FORMULA USED FOR CALCULATING THIS ERROR BOUND IS GIVEN BY ([3], [4], [5]):

$$\text{NORM}(DX) / \text{NORM}(X) \leq P / (1 - P),$$
 WHEREBY:  $P = Q * \text{NORM}(C) / (1 + Q * \text{NORM}(C)),$   
 $Q = G * (.75 * N ** 3 + 4.5 * N ** 2) * \text{EPS} + \text{EPSA},$   
 C IS THE CALCULATED INVERSE OF THE MATRIX,  
 G THE UPPER BOUND FOR THE GROWTH DURING GAUSSIAN ELIMINATION, AS DELIVERED BY GSSELM (THIS SECTION),  
 N THE ORDER OF THE MATRIX,  
 EPSA AN UPPER BOUND FOR THE RELATIVE ERROR IN THE MATRIX ELEMENTS,  
 EPS THE MACHINE PRECISION AND  
 NORM(.) DENOTES THE 1-NORM.

EXAMPLE OF USE: SEE GSSSOLERB (SECTION 3.1.1.1.1.1.3).

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SUBSECTION: GSSERB

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" GSSERB(A, N, AUX, RI, CI); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX; "INTEGER" "ARRAY" RI, CI;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE MATRIX TO BE DECOMPOSED;  
 EXIT: THE CALCULATED LOWER-TRIANGULAR MATRIX AND UNIT UPPER TRIANGULAR MATRIX, WITH ITS UNIT DIAGONAL OMITTED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[0:11];  
 ENTRY: (SEE ALSO GSSELM IN THIS SECTION);  
 AUX[0]: THE MACHINE PRECISION;  
 AUX[2]: A RELATIVE TOLERANCE;  
 AUX[4]: A VALUE WHICH IS USED FOR CONTROLLING PIVOTING;  
 AUX[6]: AN UPPER BOUND FOR THE RELATIVE PRECISION OF THE MATRIX ELEMENTS;  
 EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED, THEN AUX[1] EQUALS 1 IF THE DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R IS POSITIVE, ELSE AUX[1] = -1;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED;  
 AUX[5]: THE MODULUS OF AN ELEMENT, WHICH IS OF MAXIMUM ABSOLUTE VALUE FOR THE MATRIX GIVEN IN ARRAY A;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH;  
 AUX[9]: IF AUX[3] = N, THEN AUX[9] WILL EQUAL THE 1-NORM OF THE INVERSE MATRIX, ELSE AUX[9] WILL BE UNDEFINED;  
 AUX[11]: IF AUX[3] = N, THEN THE VALUE OF AUX[11] WILL BE A ROUGH UPPER BOUND FOR THE RELATIVE ERROR IN THE SOLUTION OF LINEAR SYSTEMS WITH A MATRIX AS GIVEN IN ARRAY A, ELSE AUX[11] WILL BE UNDEFINED; IF NO USE CAN BE MADE OF THE FORMULA FOR THE ERROR BOUND AS GIVEN ABOVE (SUBSECTION ERBELM), BECAUSE OF A VERY BAD CONDITION OF THE MATRIX, THEN AUX[11] := -1;

RI: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" RI[1:N];  
 EXIT: THE PIVOTAL ROW INDICES.

CI: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" CI[1:N];  
 EXIT: THE PIVOTAL COLUMN INDICES.

PROCEDURES USED:

GSSELM = CP34231,  
 ONENRMINV = CP34240,  
 ERBELM = CP34241.

SECTION: 3.1.1.1.1.1.1

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RUNNING TIME: PROPORTIONAL TO  $N^{**}3$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

GSSERB USES GSSELM (THIS SECTION) TO PERFORM THE TRIANGULAR DECOMPOSITION OF THE MATRIX GIVEN IN ARRAY A AND ERBELM AND ONENRMINV (THIS SECTION) TO CALCULATE AN UPPER BOUND FOR THE RELATIVE ERROR IN THE SOLUTION OF LINEAR SYSTEMS WITH A MATRIX AS GIVEN IN ARRAY A; IF  $AUX[3] < N$ , THEN THE EFFECT OF GSSERB IS MERELY THAT OF GSSELM.

EXAMPLE OF USE: SEE GSSSOLERB (SECTION 3.1.1.1.1.1.3).

SUBSECTION: GSSNRI .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" GSSNRI(A, N, AUX, RI, CI); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX; "INTEGER" "ARRAY" RI, CI;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE MATRIX TO BE DECOMPOSED;  
 EXIT: THE CALCULATED LOWER-TRIANGULAR MATRIX AND UNIT UPPER TRIANGULAR MATRIX, WITH ITS DIAGONAL OMITTED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[1:9];  
 ENTRY: (SEE ALSO GSSELM IN THIS SECTION);  
 AUX[2]: A RELATIVE TOLERANCE;  
 AUX[4]: A VALUE USED FOR CONTROLLING PIVOTING;  
 EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED, THEN AUX[1] EQUALS 1 IF THE DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R IS POSITIVE, ELSE  $AUX[1] = -1$ ;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED;  
 AUX[5]: THE MODULUS OF AN ELEMENT, WHICH IS OF MAXIMUM ABSOLUTE VALUE FOR THE MATRIX GIVEN IN ARRAY A;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH;  
 AUX[9]: IF  $AUX[3] = N$ , THEN AUX[9] WILL EQUAL THE 1-NORM OF THE INVERSE MATRIX, ELSE AUX[9] WILL BE UNDEFINED;

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RI:    <ARRAY IDENTIFIER>;
        "INTEGER" "ARRAY" RI [1:N];
        EXIT: THE PIVOTAL ROW INDICES,
CI:    <ARRAY IDENTIFIER>;
        "INTEGER" "ARRAY" CI [1:N];
        EXIT: THE PIVOTAL COLUMN INDICES,

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PROCEDURES USED:

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GSSELM      = CP34231,
ONENRMINV   = CP34240.

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RUNNING TIME: PROPORTIONAL TO  $N^{**} 3$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

GSSNRI USES GSSELM (THIS SECTION) TO PERFORM THE TRIANGULAR DECOMPOSITION OF THE MATRIX GIVEN IN ARRAY A AND ONENRMINV (THIS SECTION) TO CALCULATE THE 1-NORM OF THE INVERSE MATRIX; IF  $AUX[3] < N$ , THEN THE EFFECT OF GSSNRI IS MERELY THAT OF GSSELM (THIS SECTION).

EXAMPLE OF USE: SEE GSSITISOLERB (SECTION 3.1.1.1.1.1.5).

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## SOURCE TEXT(S):

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"CODE" 34300;
"PROCEDURE" DEC(A, N, AUX, P); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX; "INTEGER" "ARRAY" P;
"BEGIN" "INTEGER" I, K, K1, PK, D;
  "REAL" R, S, EPS;
  "ARRAY" V[1:N];
  "REAL" "PROCEDURE" MATMAT(L, U, I, J, A, B); "CODE" 34013;
  "REAL" "PROCEDURE" MATTAM(L, U, I, J, A, B); "CODE" 34015;
  "PROCEDURE" ICHROW(L, U, I, J, A); "CODE" 34032;
  R := -1;
  "FOR" I := 1 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" S := SQRT(MATTAM(1, N, I, I, A, A));
    "IF" S > R "THEN" R := S; V[I] := 1/S
  "END";
  EPS := AUX[2] * R; D := 1;
  "FOR" K := 1 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" R := -1; K1 := K - 1;
    "FOR" I := K "STEP" 1 "UNTIL" N "DO"
    "BEGIN" A[I, K] := A[I, K] - MATMAT(1, K1, I, K, A, A);
      S := ABS(A[I, K]) * V[I]; "IF" S > R "THEN"
      "BEGIN" R := S; PK := I "END"
    "END" LOWER;
    P[K] := PK; V[PK] := V[K]; S := A[PK, K];
    "IF" ABS(S) < EPS "THEN" "GOTO" END;
    "IF" S < 0 "THEN" D := -D; "IF" PK /= K "THEN"
    "BEGIN" D := -D; ICHROW(1, N, K, PK, A) "END";
    "FOR" I := K + 1 "STEP" 1 "UNTIL" N "DO"
    A[K, I] := (A[K, I] - MATMAT(1, K1, K, I, A, A)) / S
  "END" LU;
  K := N + 1;
  END: AUX[1] := D; AUX[3] := K - 1
"END" DEC;
"EOB"

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"CODE" 34231;
"PROCEDURE" GSSELM(A, N, AUX, RI, CI); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX;
"INTEGER" "ARRAY" RI, CI;
"BEGIN" "INTEGER" I, J, P, Q, R, R1, JPIV, RANK, SIGNDT;
  "REAL" CRIT, PIVOT, RGROW, MAX, AID, MAX1, EPS;
  "BOOLEAN" PARTIAL;
  "PROCEDURE" ELMROW(L, U, I, J, A, B, X); "CODE" 34024;
  "INTEGER" "PROCEDURE" MAXELMROW(L, U, I, J, A, B, X);
  "CODE" 34025;
  "PROCEDURE" ICHCOL(L, U, I, J, A); "CODE" 34031;
  "PROCEDURE" ICHROW(L, U, I, J, A); "CODE" 34032;

```

"COMMENT"

SECTION: 3.1.1.1.1.1.1

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```

"PROCEDURE" ROWCST(L, U, I, A, X); "CODE" 31132;
"REAL" "PROCEDURE" MAXMAT(LR, UR, LC, UC, I, J, A);
"CODE" 34230;
AUX[5] := RGROW := MAXMAT(1, N, 1, N, I, J, A);
CRIT := N * RGROW * AUX[4]; EPS := RGROW * AUX[2]; MAX := 0;
RANK := N; SIGNDET := 1; PARTIAL := RGROW * 0;
"FOR" Q := 1 "STEP" 1 "UNTIL" N "DO" "IF" Q * = J "THEN"
"BEGIN" AID := ABS(A[I, Q]);
  "IF" AID > MAX "THEN" MAX := AID
"END";
RGROW := RGROW + MAX;
"FOR" R := 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" R1 := R + 1; "IF" I * = R "THEN"
  "BEGIN" SIGNDET := - SIGNDET; ICHROW(1, N, R, I, A) "END";
  "IF" J * = R "THEN"
  "BEGIN" SIGNDET := - SIGNDET; ICHCOL(1, N, R, J, A) "END";
  RI[R] := I; CI[R] := J; PIVOT := A[R, R];
  "IF" PIVOT < 0 "THEN" SIGNDET := - SIGNDET;
  "IF" PARTIAL "THEN"
  "BEGIN" MAX := MAX1 := 0; J := R1;
    ROWCST(R1, N, R, A, 1 / PIVOT);
    "FOR" P := R1 "STEP" 1 "UNTIL" N "DO"
    "BEGIN" ELMROW(R1, N, P, R, A, A, = A[P, R]);
      AID := ABS(A[P, R]); "IF" MAX < AID "THEN"
      "BEGIN" MAX := AID; I := P "END";
    "END";
    "FOR" Q := R1 + 1 "STEP" 1 "UNTIL" N "DO"
    "BEGIN" AID := ABS(A[I, Q]);
      "IF" MAX1 < AID "THEN" MAX1 := AID
    "END";
    AID := RGROW; RGROW := RGROW + MAX1;
    "IF" RGROW > CRIT "OR" MAX < EPS "THEN"
    "BEGIN" PARTIAL := "FALSE"; RGROW := AID;
      MAX := MAXMAT(R1, N, R1, N, I, J, A)
    "END"
  "END" PARTIAL PIVOTINGSTEP
"ELSE"
"BEGIN" "IF" MAX <= EPS "THEN"
  "BEGIN" RANK := R - 1;
    "IF" PIVOT < 0 "THEN" SIGNDET := - SIGNDET; "GOTO" OUT
  "END";
  MAX := - 1;
  ROWCST(R1, N, R, A, 1 / PIVOT);
  "FOR" P := R1 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" JPIV := MAXELMROW(R1, N, P, R, A, A, = A[P, R]);
    AID := ABS(A[P, JPIV]); "IF" MAX < AID "THEN"
    "BEGIN" MAX := AID; I := P; J := JPIV "END"
  "END";
  "IF" RGROW < MAX "THEN" RGROW := MAX
"END" COMPLETE PIVOTINGSTEP
"END" ELIMINATIONSTEP;
OUT: AUX[1] := SIGNDET; AUX[3] := RANK; AUX[7] := RGROW
"END" GSSEL;
"EQP"

```

SECTION: 3.1.1.1.1.1.1

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```

"CODE" 34240;
"REAL" "PROCEDURE" ONENRMINV(A, N); "VALUE" N; "INTEGER" N;
"ARRAY" A;
"BEGIN" "INTEGER" I, J;
"REAL" NORM, MAX, AID;
"ARRAY" Y[I:N];
"REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
NORM:= 0;
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO" Y[I]:= "IF" I < J
"THEN" 0 "ELSE" "IF" I = J "THEN" 1 / A[I,I] "ELSE"
= MATVEC(J, I = 1, I, A, Y) / A[I,I];
MAX:= 0;
"FOR" I:= N "STEP" = 1 "UNTIL" 1 "DO"
"BEGIN" AID:= Y[I]:= Y[I] - MATVEC(I + 1, N, I, A, Y);
MAX:= MAX + ABS(AID)
"END";
"IF" NORM < MAX "THEN" NORM:= MAX
"END";
ONENRMINV:= NORM
"END" ONENRMINV;
"EOP"

"CODE" 34241;
"PROCEDURE" ERBELM(N, AUX, NRMINV); "VALUE" N, NRMINV;
"INTEGER" N; "REAL" NRMINV;
"ARRAY" AUX;
"BEGIN" "REAL" AID, EPS;
EPS:= AUX[0]; AID:= (1.06 * EPS * (.75 * N + 4.5) * N ** 2
* AUX[7] + AUX[5] * AUX[6]) * NRMINV;
AUX[11]:= "IF" 2 * AID >= (1 - EPS) "THEN" = 1 "ELSE"
AID / (1 - 2 * AID); AUX[9]:= NRMINV
"END" ERBELM;
"EOP"

"CODE" 34242;
"PROCEDURE" GSSERB(A, N, AUX, RI, CI); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX;
"INTEGER" "ARRAY" RI, CI;
"BEGIN" "PROCEDURE" GSSELM(A, N, AUX, RI, CI); "CODE" 34231;
"REAL" "PROCEDURE" ONENRMINV(A, N); "CODE" 34240;
"PROCEDURE" ERBELM(N, AUX, NRMINV); "CODE" 34241;
GSSELM(A, N, AUX, RI, CI);
"IF" AUX[3] = N "THEN" ERBELM(N, AUX, ONENRMINV(A, N))
"END" GSSERB;
"EOP"

"CODE" 34252;
"PROCEDURE" GSSNRI(A, N, AUX, RI, CI); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX;
"INTEGER" "ARRAY" RI, CI;
"BEGIN" "PROCEDURE" GSSELM(A, N, AUX, RI, CI); "CODE" 34231;
"REAL" "PROCEDURE" ONENRMINV(A, N); "CODE" 34240;
GSSELM(A, N, AUX, RI, CI);
"IF" AUX[3] = N "THEN" AUX[9]:= ONENRMINV(A, N)
"END" GSSNRI;
"EOP"

```

SECTION: 3.1.1.1.1.1.2

(MAY 1974)

PAGE 1

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CONTRIBUTOR: J.C.P. BUS AND P. A. BRENTJES,

INSTITUTE: MATHEMATICAL CENTRE,

RECEIVED: 730831.

## BRIEF DESCRIPTION:

THIS SECTION CONTAINS A PROCEDURE FOR CALCULATING THE DETERMINANT OF A TRIANGULAR DECOMPOSED MATRIX;

## KEYWORDS:

DETERMINANT.

## CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:

"REAL" "PROCEDURE" DETERM(A, N, SIGN); "VALUE" N, SIGN;  
"INTEGER" N, SIGN; "ARRAY" A;

DETERM: DELIVERS THE CALCULATED VALUE OF THE DETERMINANT OF THE MATRIX;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" A[1:N, 1:N];

ENTRY: THE DIAGONAL ELEMENTS OF THE LOWER-TRIANGULAR MATRIX L, OBTAINED BY TRIANGULAR DECOMPOSITION OF THE MATRIX, HAS TO BE GIVEN IN A[I,I], I= 1, ..., N;

N: &lt;ARITHMETIC EXPRESSION&gt;;

THE ORDER OF THE MATRIX, WHOSE DETERMINANT HAS TO BE CALCULATED;

SIGN: &lt;ARITHMETIC EXPRESSION&gt;;

ENTRY: IF THE DETERMINANT OF THE MATRIX IS POSITIVE THEN THE VALUE OF SIGN SHOULD BE +1, ELSE -1; THIS VALUE IS DELIVERED BY GSSELM OR DEC IN AUX[1], (SECTION 3.1.1.1.1.1.1).

PROCEDURES USED: NONE.



SECTION: 3.1.1.1.1.1.2

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RUNNING TIME: PROPORTIONAL TO N.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

A LOWER-TRIANGULAR MATRIX L HAS TO BE GIVEN, SUCH THAT FOR SOME UNIT UPPER-TRIANGULAR MATRIX U THE PRODUCT LU EQUALS THE MATRIX (WITH PERMUTED ROWS AND COLUMNS); THE SIGN OF THE DETERMINANT ALSO HAS TO BE GIVEN; THESE DATA ARE DELIVERED IN THE MATRIX AND AUX[1] BY THE PROCEDURES GSSELM OR DEC (SECTION 3.1.1.1.1.1.1) AND THE PROCEDURES GSSERB, GSSNRI (SECTION 3.1.1.1.1.1.1), DECSOL, GSSSOL, GSSSOLERB (SECTION 3.1.1.1.1.1.3), GSSITISOL AND GSSITISOLERB (SECTION 3.1.1.1.1.1.5), WHICH MAKE USE OF GSSELM OR DEC.

THE CALCULATION OF THE DETERMINANT IS DONE STRAIGHT ON BY CALCULATING THE PRODUCT OF THE DIAGONAL ELEMENTS OF THE LOWER-TRIANGULAR MATRIX GIVEN IN ARRAY A; THE USER IS WARNED, THAT OVERFLOW MAY OCCUR IF THE ORDER OF THE MATRIX IS LARGE.

EXAMPLE OF USE:

THE DETERMINANT OF THE FOURTH ORDER SEGMENT OF THE HILBERT MATRIX MAY BE OBTAINED BY THE FOLLOWING PROGRAM:

```
"BEGIN" "INTEGER" I, J; "REAL" D; "INTEGER" "ARRAY" RI, CI[1:4];
  "ARRAY" A[1:4, 1:4], AUX[1:7];
  "PROCEDURE" GSSELM(A, N, AUX, RI, CI); "CODE" 34231;
  "REAL" "PROCEDURE" DETERM(A, N, SIGN); "CODE" 34303;
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO" A[I, J]:= 1 / (I + J - 1);
  AUX[2]:= "-14; AUX[4]:= 8;
  GSSELM(A, 4, AUX, RI, CI);
  D:= "IF" AUX[3] = 4 "THEN" DETERM(A, 4, AUX[1]) "ELSE" 0;
  OUTPUT(71, "(""("DETERMINANT =)"B+.15D"+3D").", D)
"END"
```

RESULT:

DETERMINANT = +.165343915345370"-006

SOURCE TEXT(S):

```
"CODE" 34303;
"REAL" "PROCEDURE" DETERM(A, N, SIGN); "VALUE" N, SIGN;
"INTEGER" N, SIGN; "ARRAY" A;
"BEGIN" "INTEGER" I; "REAL" DET;
  DET:= 1;
  "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO" DET:= A[I, I] * DET;
  DETERM:= SIGN * ABS(DET)
"END" DETERM;
"EOF"
```

SECTION: 3.1.1.1.1.1.3

(MAY 1974)

PAGE 1

AUTHORS: J. C. P. BUS AND T. J. DEKKER.

CONTRIBUTOR: J.C.P. BUS AND P. A. BEENTJES.

INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED: 730915.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS FIVE PROCEDURES:  
 SOL SOLVES THE LINEAR SYSTEM WHOSE MATRIX HAS BEEN TRIANGULARLY  
 DECOMPOSED BY DEC;  
 DECSOL SOLVES A LINEAR SYSTEM WHOSE ORDER IS SMALL RELATIVE TO THE  
 NUMBER OF BINARY DIGITS IN THE NUMBER REPRESENTATION;  
 SOLELM SOLVES A LINEAR SYSTEM WHOSE MATRIX HAS BEEN TRIANGULARLY  
 DECOMPOSED BY GSSELM OR GSSERB (SECTION 3.1.1.1.1.1.).  
 GSSSOL SOLVES A LINEAR SYSTEM;  
 GSSSOLERB SOLVES A LINEAR SYSTEM AND CALCULATES A ROUGH  
 UPPERBOUND FOR THE RELATIVE ERROR IN THE CALCULATED SOLUTION;

THE  
 DIFFERENCE BETWEEN DECSOL ON THE ONE SIDE AND GSSSOL AND GSSSOLERB  
 ON THE OTHER SIDE LIES IN THE METHOD USED FOR TRIANGULAR  
 DECOMPOSITION, PARTICULARLY IN THE PIVOTING STRATEGY; DECSOL USES  
 DEC, GSSSOL AND GSSSOLERB USE GSSELM TO PERFORM THE TRIANGULAR  
 DECOMPOSITION (SECTION 3.1.1.1.1.1.); SINCE, IN EXCEPTIONAL CASES,  
 DEC MAY YIELD USELESS RESULTS, ONE IS ADVISED TO USE GSSSOL OR  
 GSSSOLERB; HOWEVER, IF THE ORDER OF THE LINEAR SYSTEM IS VERY SMALL  
 RELATIVE TO THE NUMBER OF BINARY DIGITS IN THE NUMBER  
 REPRESENTATION, THEN DECSOL ALSO MAY BE USED.

KEYWORDS:

ALGEBRAIC EQUATIONS,  
 LINEAR SYSTEMS.

SECTION: 3.1.1.1.1.1.5

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SUBSECTION: SOL .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" SOL(A, N, P, B); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, B; "INTEGER" "ARRAY" P;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX OF  
 THE LINEAR SYSTEM AS PRODUCED BY DEC (SECTION  
 3.1.1.1.1.1.1);  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;  
 P: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" P[1:N];  
 ENTRY: THE PIVOTAL INDICES, AS PRODUCED BY DEC.  
 B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: THE SOLUTION OF THE LINEAR SYSTEM,

PROCEDURES USED:

MATVEC = CP34011.

RUNNING TIME: PROPORTIONAL TO  $N \star \star 2$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SOL SHOULD BE CALLED AFTER DEC (SECTION 3.1.1.1.1.1.1) AND SOLVES  
 THE LINEAR SYSTEM WITH A MATRIX, WHOSE TRIANGULARLY DECOMPOSED FORM  
 AS PRODUCED BY DEC IS GIVEN IN ARRAY A, AND A RIGHT-HAND SIDE AS  
 GIVEN IN ARRAY B; SOL LEAVES A AND P UNALTERED, SO, AFTER ONE CALL  
 OF DEC, SEVERAL CALLS OF SOL MAY FOLLOW FOR SOLVING SEVERAL SYSTEMS  
 HAVING THE SAME MATRIX BUT DIFFERENT RIGHT-HAND SIDES,

EXAMPLE OF USE: SEE DECSOL (THIS SECTION),

SUBSECTION: DECSOL .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" DECSOL(A, N, AUX, B); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE N-TH ORDER MATRIX;  
 EXIT: THE CALCULATED LOWER-TRIANGULAR MATRIX AND UNIT  
 UPPERTRIANGULAR MATRIX WITH ITS UNIT DIAGONAL OMITTED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[1:3];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R  
 IS POSITIVE, ELSE AUX[1] = -1;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 AUX[3] < N THEN THE PROCESS IS TERMINATED AND NO  
 SOLUTION WILL BE CALCULATED;

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: IF AUX[3] = N, THEN THE CALCULATED SOLUTION OF THE  
 LINEAR SYSTEM IS OVERWRITTEN ON B, ELSE B REMAINS  
 UNALTERED.

PROCEDURES USED:

DEC = CP34300,  
 SOL = CP34051.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: DECSOL DECLARES AN AUXILIARY ARRAY OF TYPE  
 INTEGER AND ORDER N.

RUNNING TIME: PROPORTIONAL TO N \*\* 3.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

DECSOL USES DEC TO PERFORM THE TRIANGULAR DECOMPOSITION OF THE MATRIX AND SOL TO CALCULATE THE SOLUTION WITH FORWARD AND BACK SUBSTITUTION; SINCE DECSOL MAY YIELD USELESS RESULTS, EVEN FOR WELL-CONDITIONED MATRICES (SEE DEC, SECTION 3.1.1.1.1.1), DECSOL SHOULD ONLY BE USED IF THE ORDER OF THE MATRIX IS SMALL RELATIVE TO THE NUMBER OF BINARY DIGITS IN THE NUMBER REPRESENTATION; IF  $AUX[3] < N$ , THEN THE EFFECT OF DECSOL IS MERELY THAT OF DEC.

## EXAMPLE OF USE:

LET A BE THE FOURTH ORDER SEGMENT OF THE HILBERT MATRIX AND B THE THIRD COLUMN OF A, THEN THE SOLUTION OF THE LINEAR SYSTEM  $AX = B$  IS GIVEN BY THE THIRD UNIT VECTOR AND MAY BE CALCULATED BY THE FOLLOWING PROGRAM:

```
"BEGIN" "INTEGER" I, J;
  "ARRAY" A[1:4, 1:4], B[1:4], AUX[1:3];
  "PROCEDURE" DECSOL(A, N, AUX, B); "CODE" 34301;
  "PROCEDURE" LIST(ITEM); "PROCEDURE" ITEM;
  "BEGIN" "INTEGER" I;
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO" ITEM(B[I]);
    "FOR" I:= 1 "STEP" 2 "UNTIL" 3 "DO" ITEM(AUX[I])
  "END" LIST;
  "PROCEDURE" LAYOUT;
  FORMAT("( * , (" SOLUTION: ") "B+,15D"+3D,/,3(10B+,15D"+3D,/,),
  ("SIGN(DET) = ")"+D,/,("NUMBER OF ELIMINATIONSTEPS = ")"+
  +D)");

  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    A[I,J]:= 1 / (I + J - 1); B[I]:= A[I,3]
  "END";
  AUX[2]:= "-14;
  DECSOL(A, 4, AUX, B);
  OUTLIST(71, LAYOUT, LIST)
"END"
```

## RESULTS:

```
SOLUTION: +,0000000000000000"+000
           +,0000000000000000"+000
           +,1000000000000000"+001
           +,0000000000000000"+000
SIGN(DET) = +1
NUMBER OF ELIMINATIONSTEPS = +4
```

SECTION: 3.1.1.1.1.3

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SUBSECTION: SOLELM .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" SOLELM(A, N, RI, CI, B); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, B; "INTEGER" "ARRAY" RI, CI;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX OF  
 THE LINEAR SYSTEM AS PRODUCED BY GSSELM (SECTION  
 3.1.1.1.1.1);  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;  
 RI: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" RI[1:N];  
 ENTRY: THE PIVOTAL ROW INDICES, AS PRODUCED BY GSSELM;  
 CI: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" CI[1:N];  
 ENTRY: THE PIVOTAL COLUMN INDICES, AS PRODUCED BY GSSELM;  
 B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: THE SOLUTION OF THE LINEAR SYSTEM.

PROCEDURES USED:

SOL = CP34051.

RUNNING TIME: PROPORTIONAL TO  $N ** 2$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SOLELM SHOULD BE CALLED AFTER GSSELM OR GSSERB (SECTION 3.1.1.1.1.1) AND SOLVES THE LINEAR SYSTEM WITH THE MATRIX, WHOSE TRIANGULARLY DECOMPOSED FORM AS PRODUCED BY GSSELM IS GIVEN IN ARRAY A, AND A RIGHT-HAND SIDE AS GIVEN IN ARRAY B; SOLELM LEAVES A, RI AND CI UNALTERED, SO, AFTER ONE CALL OF GSSELM OR GSSERB, SEVERAL CALLS OF SOLELM MAY FOLLOW FOR SOLVING SEVERAL SYSTEMS HAVING THE SAME MATRIX BUT DIFFERENT RIGHT-HAND SIDES.

EXAMPLE OF USE: SEE GSSSOL OR GSSSOLERB (THIS SECTION).

SUBSECTION: GSSSOL

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" GSSSOL(A, N, AUX, B); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE N-TH ORDER MATRIX;  
 EXIT: THE CALCULATED LOWER-TRIANGULAR MATRIX AND UNIT  
 UPPERTRIANGULAR MATRIX WITH ITS UNIT DIAGONAL OMITTED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[1:7];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 AUX[4]: A VALUE WHICH IS USED FOR CONTROLLING PIVOTING (SEE  
 GSSELM, SECTION 3.1.1.1.1.1.1);  
 EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R  
 IS POSITIVE, ELSE AUX[1] = -1;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 AUX[3] < N THEN THE PROCESS IS TERMINATED AND NO  
 SOLUTION WILL HAVE BEEN CALCULATED;  
 AUX[5]: THE MODULUS OF AN ELEMENT WHICH IS OF MAXIMUM  
 ABSOLUTE VALUE FOR THE MATRIX GIVEN IN ARRAY A;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH (SEE GSSELM, SECTION  
 3.1.1.1.1.1.1);

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: IF AUX[3] = N, THEN THE CALCULATED SOLUTION OF THE  
 LINEAR SYSTEM IS OVERWRITTEN ON B, ELSE B REMAINS  
 UNALTERED.

PROCEDURES USED:

SOLELM = CP34061,  
 GSSELM = CP34231.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: GSSSOL DECLARES TWO AUXILIARY ARRAYS OF  
 TYPE INTEGER AND ORDER N.

SECTION: 3.1.1.1.1.1.3

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RUNNING TIME: PROPORTIONAL TO  $N^{**}3$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

GSSSOL USES GSSFLM (SECTION 3.1.1.1.1.1) TO PERFORM A TRIANGULAR DECOMPOSITION OF THE MATRIX AND SOLELM (THIS SECTION) TO CALCULATE THE SOLUTION OF THE GIVEN LINEAR SYSTEM; IF  $AUX[3] < N$ , THEN THE EFFECT OF GSSSOL IS MERELY THAT OF GSSELM.

EXAMPLE OF USE:

LET A BE THE FOURTH ORDER SEGMENT OF THE HILBERT MATRIX AND B THE THIRD COLUMN OF A, THEN THE SOLUTION OF THE LINEAR SYSTEM  $AX = B$  IS GIVEN BY THE THIRD UNIT VECTOR AND MAY BE CALCULATED BY THE FOLLOWING PROGRAM:

```
"BEGIN" "INTEGER" I, J;
  "ARRAY" A[1:4, 1:4], B[1:4], AUX[1:7];
  "PROCEDURE" GSSSOL(A, N, AUX, B); "CODE" 34232;
  "PROCEDURE" LIST(ITEM); "PROCEDURE" ITEM;
  "BEGIN" "INTEGER" I;
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO" ITEM(B[I]);
    "FOR" I:= 1 "STEP" 2 "UNTIL" 7 "DO" ITEM(AUX[I]);
  "END" LIST;
  "PROCEDURE" LAYOUT;
  FORMAT("(*, ("SOLUTION:")"B+.15D"+3D,/,3(10B+.15D"+3D,/,),
    ("SIGN(DET) = ")"+D,/,("NUMBER OF ELIMINATIONSTEPS = ")"+
    +D,/,("MAX(ABS(A[I,J]))= ")"+.15D"+3D,/,
    ("UPPER BOUND GROWTH: ")"+.15D"+3D)");

  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    A[I,J]:= 1 / (I + J - 1); B[I]:= A[I,3]
  "END";
  AUX[2]:= "-14; AUX[4]:= 8;
  GSSSOL(A, 4, AUX, B);
  OUTLIST(71, LAYOUT, LIST)
"END"
```

RESULTS:

```
SOLUTION: +.888178419700120"-014
          -.497379915032070"-013
          +.1000000000000010"+001
          +.0000000000000000"+000
SIGN(DET) = +1
NUMBER OF ELIMINATIONSTEPS = +4
MAX(ABS(A[I,J]))= +.1000000000000000"+001
UPPER BOUND GROWTH: +.159619047619050"+001
```



## SUBSECTION: GSSSOLERB.

## CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" GSSSOLERB(A, N, AUX, B); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX, B;

## THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE N-TH ORDER MATRIX;  
 EXIT: THE CALCULATED LOWER-TRIANGULAR MATRIX AND UNIT  
 UPPERTRIANGULAR MATRIX WITH ITS UNIT DIAGONAL OMITTED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[0:11];  
 ENTRY:  
 AUX[0]: THE MACHINE PRECISION;  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 AUX[4]: A VALUE WHICH IS USED FOR CONTROLLING PIVOTING (SEE  
 GSSELM, SECTION 3.1.1.1.1.1);  
 AUX[6]: AN UPPER BOUND FOR THE RELATIVE PRECISION OF THE  
 GIVEN MATRIX ELEMENTS;  
 EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R  
 IS POSITIVE, ELSE AUX[1] = -1;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 AUX[3] < N THEN THE PROCESS IS TERMINATED AND NO  
 SOLUTION OR ERROR BOUND WILL HAVE BEEN CALCULATED;  
 AUX[5]: THE MODULUS OF AN ELEMENT WHICH IS OF MAXIMUM  
 ABSOLUTE VALUE FOR THE MATRIX GIVEN IN ARRAY A;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH (SEE GSSELM, SECTION  
 3.1.1.1.1.1);  
 AUX[9]: IF AUX[3] = N, THEN AUX[9] WILL EQUAL THE 1-NORM OF  
 THE INVERSE MATRIX, ELSE AUX[9] WILL BE UNDEFINED;  
 AUX[11]: IF AUX[3] = N THEN THE VALUE OF AUX[11] WILL BE A  
 ROUGH UPPER BOUND FOR THE RELATIVE ERROR IN THE  
 CALCULATED SOLUTION OF THE GIVEN LINEAR SYSTEM,  
 ELSE AUX[11] WILL BE UNDEFINED; IF NO USE CAN BE  
 MADE OF THE FORMULA FOR THE ERROR BOUND AS GIVEN IN  
 SECTION 3.1.1.1.1.1 (SUBSECTION ERBELM), BECAUSE  
 OF A VERY BAD CONDITION OF THE MATRIX, THEN  
 AUX[11] := -1;

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: IF AUX[3] = N, THEN THE CALCULATED SOLUTION OF THE  
 LINEAR SYSTEM, ELSE B REMAINS UNALTERED.

## PROCEDURES USED:

SOLELM = CP34061,  
GSSSERB = CP34242.

## REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: GSSSOLERB DECLARES TWO AUXILIARY ARRAYS OF TYPE INTEGER AND ORDER N.

RUNNING TIME: PROPORTIONAL TO  $N ** 3$ .

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

GSSSOLERB USES GSSSERB (SECTION 3.1.1.1.1.1) TO PERFORM THE TRIANGULAR DECOMPOSITION OF THE MATRIX AND TO CALCULATE AN UPPER BOUND FOR THE RELATIVE ERROR IN THE CALCULATED SOLUTION OF THE GIVEN LINEAR SYSTEM, AND SOLELM (THIS SECTION) TO CALCULATE THIS SOLUTION; IF  $AUX[3] < N$ , THEN THE EFFECT OF GSSSOLERB IS MERELY THAT OF GSSELM (SECTION 3.1.1.1.1.1).

## EXAMPLE OF USE:

LET A BE THE FOURTH ORDER SEGMENT OF THE HILBERT MATRIX AND B THE THIRD COLUMN OF A, THEN THE SOLUTION OF THE LINEAR SYSTEM  $AX = B$  IS GIVEN BY THE THIRD UNIT VECTOR AND THIS SOLUTION, AS WELL AS AN UPPER BOUND FOR THE RELATIVE ERROR IN THE CALCULATED ONE, MAY BE OBTAINED BY THE FOLLOWING PROGRAM:

```
"BEGIN" "INTEGER" I, J;
  "ARRAY" A[1:4, 1:4], B[1:4], AUX[0:11];
  "PROCEDURE" GSSSOLERB(A, N, AUX, B); "CODE" 34243;
  "PROCEDURE" LIST(ITEM); "PROCEDURE" ITEM;
  "BEGIN" "INTEGER" I;
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO" ITEM(B[I]);
    "FOR" I:= 1 "STEP" 2 "UNTIL" 11 "DO" ITEM(AUX[I])
  "END" LIST;
  "PROCEDURE" LAYOUT;
  FORMAT("(*, ("SOLUTION:")"B+.15D"+3D,/,3(10B+.15D"+3D,/,),
  ("SIGN(DET) = ")"+D,/,("NUMBER OF ELIMINATIONSTEPS = ")"+
  +D,/,("MAX(ABS(A[I,J]))= ")"+.15D"+3D,/,
  ("UPPER BOUND GROWTH: ")"+.15D"+3D,/,
  ("||-NORM OF THE INVERSE MATRIX:")"B+.15D"+3D,/,
  ("UPPER BOUND REL. ERR. IN THE CALC. SOL.")"
  B+.15D"+3D")");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    A[I,J]:= 1 / (I + J - 1); B[I]:= A[I,3]
  "END";
  AUX[0]:= AUX[2]:= "-14; AUX[4]:= 8; AUX[6]:= "-14;
  GSSSOLERB(A, 4, AUX, B);
  OUTLIST(71, LAYOUT, LIST)
"END"
```

RESULTS:

SOLUTION: +.888178419700120"-014  
 -.497379915032070"-013  
 +.1000000000000010"+001  
 +.0000000000000000"+000  
 SIGN(DET) = +1  
 NUMBER OF ELIMINATIONSTEPS = +4  
 MAX(ABS(A[I,J]))= +.1000000000000000"+001  
 UPPER BOUND GROWTH: +.159619047619050"+001  
 1-NORM OF THE INVERSE MATRIX: +.136199999998790"+005  
 UPPER BOUND REL. ERR. IN THE CALC. SOL. +.277896269157090"-007

REFERENCES:

- [1] BUS, J. C. P.,  
 LINEAR SYSTEMS WITH CALCULATION OF ERROR BOUNDS AND ITERATIVE  
 REFINEMENT (DUTCH).  
 MATHEMATICAL CENTRE, AMSTERDAM, LR 3, 4, 19 (1972).
- [2] DEKKER, T. J.,  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 1,  
 MATHEMATICAL CENTRE, AMSTERDAM, TRACT 22 (1968).

SOURCE TEXT(S):

```
"CODE" 34051;
"PROCEDURE" SOL(A, N, P, B); "VALUE" N; "INTEGER" N; "ARRAY" A, B;
"INTEGER" "ARRAY" P;
"BEGIN" "INTEGER" K, PK;
  "REAL" R;
  "REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
  "FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
    "BEGIN" R:= B[K]; PK:= P[K];
      B[K]:= (B[PK] - MATVEC(1, K - 1, K, A, B)) / A[K,K];
      "IF" PK ^= K "THEN" B[PK]:= R
    "END";
  "FOR" K:= N "STEP" - 1 "UNTIL" 1 "DO"
    B[K]:= B[K] - MATVEC(K + 1, N, K, A, B)
"END" SOL;
"EOP"
```

```

"CODE" 34301;
  "PROCEDURE" DECSOL(A, N, AUX, B); "VALUE" N; "INTEGER" N;
  "ARRAY" A, AUX, B;
  "BEGIN" "INTEGER" "ARRAY" P[1:N];
    "PROCEDURE" SOL(A, N, P, B); "CODE" 34051;
    "PROCEDURE" DEC(A, N, AUX, P); "CODE" 34300;
    DEC(A, N, AUX, P);
    "IF" AUX[3] = N "THEN" SOL(A, N, P, B)
  "END" DECSOL;
  "EOP"

"CODE" 34061;
  "PROCEDURE" SOLELM(A, N, RI, CI, B); "VALUE" N; "INTEGER" N;
  "ARRAY" A, B;
  "INTEGER" "ARRAY" RI, CI;
  "BEGIN" "INTEGER" R, CIR;
    "REAL" W;
    "PROCEDURE" SOL(A, N, P, B); "CODE" 34051;
    SOL(A, N, RI, B);
    "FOR" R:= N "STEP" - 1 "UNTIL" 1 "DO"
      "BEGIN" CIR:= CI[R]; "IF" CIR ^= R "THEN"
        "BEGIN" W:= B[R]; B[R]:= B[CIR]; B[CIR]:= W "END"
    "END"
  "END" SOLELM;
  "EOP"

"CODE" 34232;
  "PROCEDURE" GSSSOL(A, N, AUX, B); "VALUE" N; "INTEGER" N;
  "ARRAY" A, AUX, B;
  "BEGIN" "INTEGER" "ARRAY" RI, CI[1:N];
    "PROCEDURE" SOLELM(A, N, RI, CI, B); "CODE" 34061;
    "PROCEDURE" GSSELM(A, N, AUX, RI, CI); "CODE" 34231;
    GSSELM(A, N, AUX, RI, CI);
    "IF" AUX[3] = N "THEN" SOLELM(A, N, RI, CI, B)
  "END" GSSSOL;
  "EOP"

"CODE" 34243;
  "PROCEDURE" GSSSOLFRB(A, N, AUX, B); "VALUE" N; "INTEGER" N;
  "ARRAY" A, AUX, B;
  "BEGIN" "INTEGER" "ARRAY" RI, CI[1:N];
    "PROCEDURE" SOLELM(A, N, RI, CI, B); "CODE" 34061;
    "PROCEDURE" GSSERB(A, N, AUX, RI, CI); "CODE" 34242;
    GSSERB(A, N, AUX, RI, CI);
    "IF" AUX[3] = N "THEN" SOLELM(A, N, RI, CI, B)
  "END" GSSSOLFRB;
  "EOP"

```

SECTION: 3.1.1.1.1.1.4

(DECEMBER 1975)

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BRIEF DESCRIPTION:

THIS SECTION CONTAINS FIVE PROCEDURES FOR INVERSION OF MATRICES:  
INV CALCULATES THE INVERSE OF A MATRIX THAT HAS BEEN TRIANGULARLY  
DECOMPOSED BY DEC;  
DECINV CALCULATES THE INVERSE OF A MATRIX WHOSE ORDER IS SMALL  
RELATIVE TO THE NUMBER OF BINARY DIGITS IN THE NUMBER  
REPRESENTATION;  
INV1 CALCULATES THE INVERSE OF A MATRIX THAT HAS BEEN TRIANGULARLY  
DECOMPOSED BY GSSELM OR GSSERB. THE 1-NORM OF THE INVERSE MATRIX  
MIGHT ALSO BE CALCULATED  
GSSINV CALCULATES THE INVERSE OF A MATRIX;  
GSSINVERB CALCULATES THE INVERSE OF A MATRIX AND ITS 1-NORM.  
A ROUGH UPPERBOUND FOR THE RELATIVE ERROR IN THE CALCULATED INVERSE  
MATRIX IS ALSO GIVEN;

THE DIFFERENCE  
BETWEEN DECINV ON THE ONE SIDE AND GSSINV AND GSSINVERB ON THE  
OTHER SIDE LIES IN THE METHOD USED FOR TRIANGULAR DECOMPOSITION,  
PARTICULARLY IN THE PIVOTING STRATEGY; DECINV USES DEC, GSSINV AND  
GSSINVERB USE GSSELM TO PERFORM THE TRIANGULAR DECOMPOSITION; THE  
USER IS ADVISED TO USE GSSINV OR GSSINVERB (SEE SECTION  
3.1.1.1.1.1).

KEYWORDS:

MATRIX INVERSION.

SECTION: 3.1.1.1.1.1.4

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SUBSECTION: INV .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
"PROCEDURE" INV(A, N, P); "VALUE" N;  
"INTEGER" N; "ARRAY" A; "INTEGER" "ARRAY" P;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1:N, 1:N];  
ENTRY: THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX AS  
PRODUCED BY DEC (SECTION 3.1.1.1.1.1.1);  
EXIT: THE CALCULATED INVERSE MATRIX;  
N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE MATRIX;  
P: <ARRAY IDENTIFIER>;  
"INTEGER""ARRAY P[1:N];  
ENTRY: THE PIVOTAL INDICES, AS PRODUCED BY DEC;

PROCEDURES USED:

MATMAT = CP34013,  
ICHCOL = CP34031,  
DUPCOLVEC = CP31034.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: INV DECLARES AN AUXILIARY ARRAY OF TYPE  
REAL AND ORDER N.

RUNNING TIME: PROPORTIONAL TO N \*\* 3.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

INV SHOULD BE CALLED AFTER DEC (SECTION 3.1.1.1.1.1.1) AND  
CALCULATES THE INVERSE OF THE MATRIX, WHOSE TRIANGULARLY DECOMPOSED  
FORM AS PRODUCED BY DEC IS GIVEN IN ARRAY A; THE INVERSE MATRIX IS  
OVERWRITTEN ON A.

EXAMPLE OF USE: SEE DECINV (THIS SECTION).

SECTION: 3.1.1.1.1.1.4

(DECEMBER 1975)

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SUBSECTION: DECINV .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" DECINV(A, N, AUX); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE MATRIX, WHOSE INVERSE HAS TO BE CALCULATED;  
 EXIT: IF AUX[3] = N, THEN THE CALCULATED INVERSE MATRIX;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[1:3];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;

EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R  
 IS POSITIVE, ELSE AUX[1] = -1;

AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 AUX[3] < N, THEN THE PROCESS IS TERMINATED AND NO  
 INVERSE WILL HAVE BEEN CALCULATED.

PROCEDURES USED:

DEC = CP34300,  
 INV = CP34053.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: DECINV DECLARES AN AUXILIARY ARRAY OF TYPE  
 INTEGER AND ORDER N.

RUNNING TIME: PROPORTIONAL TO N \*\* 3.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

DECINV USES DEC (SECTION 3.1.1.1.1.1) TO PERFORM THE TRIANGULAR DECOMPOSITION OF A MATRIX AND INV TO CALCULATE ITS INVERSE; DECINV SHOULD ONLY BE USED IF THE ORDER OF THE MATRIX IS SMALL RELATIVE TO THE NUMBER OF BINARY DIGITS IN THE NUMBER REPRESENTATION (SEE DEC); IF AUX[3] < N, THEN THE EFFECT OF DECINV IS MERELY THAT OF DEC.

## EXAMPLE OF USE:

THE FOLLOWING PROGRAM CALCULATES THE INVERSE OF THE INPUT MATRIX AND PRINTS THE RESULTS:

```

"BEGIN"
  "ARRAY" A[1:4, 1:4], AUX[1:3];
  "PROCEDURE" DECINV(A, N, AUX); "CODE" 34302;
  "PROCEDURE" LIST(ITEM); "PROCEDURE" ITEM;
  "BEGIN" "INTEGER" I, J;
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
      "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO" ITEM(A[I,J])
  "END" LIST;
  "PROCEDURE" LAYOUT;
  FORMAT (" ("4(4B,4(B+ZDB),/),/"");

  INLIST(70, LAYOUT, LIST); AUX[2]:= "-14;
  OUTPUT(71, ("(/,"("CALCULATED INVERSE:"),/"");
  DECINV(A, 4, AUX);
  OUTLIST(71, LAYOUT, LIST);
  OUTPUT(71, ("("("AUX[1]=")B+D,/,("AUX[3]=")B+D)",
  AUX[1], AUX[3])
"END"

```

## INPUT:

+ 4	+ 2	+ 4	+ 1
+30	+20	+45	+12
+20	+15	+36	+10
+35	+28	+70	+20

## RESULTS:

CALCULATED INVERSE:			
+4	-2	+4	-1
-30	+20	-45	+12
+20	-15	+36	-10
-35	+28	-70	+20

AUX[1]= +1  
AUX[3]= +4



SECTION: 3.1.1.1.1.1.4

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SUBSECTION: INV1 .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:

"REAL" "PROCEDURE" INV1(A, N, RI, CI, WITHNORM);

"VALUE" N, WITHNORM; "INTEGER" N; "BOOLEAN" WITHNORM; "ARRAY" A;

"INTEGER" "ARRAY" RI, CI;

INV1: IF THE VALUE OF WITHNORM IS TRUE, THEN THE VALUE OF INV1  
WILL EQUAL THE 1-NORM OF THE CALCULATED INVERSE MATRIX,  
ELSE INV1:= 0;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" A[1:N, 1:N];

ENTRY: THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX AS  
PRODUCED BY GSSELM (SECTION 3.1.1.1.1.1);

EXIT: THE CALCULATED INVERSE MATRIX;

N: &lt;ARITHMETIC EXPRESSION&gt;;

THE ORDER OF THE MATRIX;

RI: &lt;ARRAY IDENTIFIER&gt;;

"INTEGER""ARRAY" RI[1:N];

ENTRY: THE PIVOTAL ROW INDICES, AS PRODUCED BY GSSELM;

CI: &lt;ARRAY IDENTIFIER&gt;;

"INTEGER""ARRAY" CI[1:N];

ENTRY: THE PIVOTAL COLUMN INDICES, AS PRODUCED BY GSSELM;

WITHNORM: &lt;BOOLEAN EXPRESSION&gt;;

IF THE VALUE OF WITHNORM IS TRUE, THEN THE 1-NORM OF THE  
INVERSE MATRIX WILL BE CALCULATED AND ASSIGNED TO INV1,

ELSE INV1:= 0;

PROCEDURES USED:

ICHROW = CP34032,

INV = CP34053.

RUNNING TIME: PROPORTIONAL TO N \*\* 3.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

INV1 SHOULD BE CALLED AFTER GSSELM OR GSSERB (SECTION  
3.1.1.1.1.1), WHICH DELIVERS THE TRIANGULARLY DECOMPOSED FORM OF A  
MATRIX; INV1 CALCULATES THE INVERSE MATRIX AND ALSO ITS 1-NORM  
MIGHT BE CALCULATED; THE INVERSE MATRIX IS OVERWRITTEN ON A.

EXAMPLE OF USE: SEE GSSINV AND GSSINVERB (THIS SECTION).

SECTION: 3.1.1.1.1.1.4

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SUBSECTION: GSSINV .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" GSSINV(A, N, AUX); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE MATRIX, WHOSE INVERSE HAS TO BE CALCULATED;  
 EXIT: IF AUX[3] = N, THEN THE CALCULATED INVERSE MATRIX;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[1:9];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 AUX[4]: A VALUE WHICH IS USED FOR CONTROLLING PIVOTING (SEE  
 GSSELM, SECTION 3.1.1.1.1.1.1);  
 EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R  
 IS POSITIVE, ELSE AUX[1] = -1;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 AUX[3] < N THEN THE PROCESS IS TERMINATED AND NO  
 SOLUTION WILL BE CALCULATED;  
 AUX[5]: THE MODULUS OF AN ELEMENT WHICH IS OF MAXIMUM  
 ABSOLUTE VALUE FOR THE MATRIX GIVEN IN ARRAY A;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH (SEE GSSELM, SECTION  
 3.1.1.1.1.1.1);  
 AUX[9]: IF AUX[3] = N, THEN AUX[9] WILL EQUAL THE 1-NORM OF  
 THE CALCULATED INVERSE MATRIX, ELSE AUX[9] WILL BE  
 UNDEFINED.

PROCEDURES USED:

INV1 = CP34235,  
 GSSELM = CP34231.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: GSSINV DECLARES TWO AUXILIARY ARRAYS OF  
 TYPE INTEGER AND ORDER N.

RUNNING TIME: PROPORTIONAL TO N \*\* 3.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

GSSINV USES GSSELM (SECTION 3.1.1.1.1.1.1) TO PERFORM A TRIANGULAR DECOMPOSITION OF THE MATRIX AND INV1 (THIS SECTION) TO CALCULATE THE INVERSE MATRIX; IF AUX[3] = N, THEN THE EFFECT OF GSSINV IS MERELY THAT OF GSSELM.

## EXAMPLE OF USE:

THE FOLLOWING PROGRAM CALCULATES THE INVERSE OF THE INPUT MATRIX AND PRINTS THE RESULTS:

```

"BEGIN"
  "ARRAY" A[1:4, 1:4], AUX[1:9];
  "PROCEDURE" GSSINV(A, N, AUX); "CODE" 34236;
  "PROCEDURE" LIST(ITEM); "PROCEDURE" ITEM;
  "BEGIN" "INTEGER" I, J;
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
      "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO" ITEM(A[I,J])
  "END" LIST;
  "PROCEDURE" LAYOUT;
  FORMAT (" ("4(4B,4(B+ZDB),/),/)" );

  INLIST(70, LAYOUT, LIST); AUX[2]:= "-14; AUX[4]:= 8;
  GSSINV(A, 4, AUX);
  OUTPUT(71, (" /, ("CALCULATED INVERSE:"), /" );
  OUTLIST(71, LAYOUT, LIST);
  OUTPUT(71, ("4B" ("AUX ELEMENTS:"), /, 2(4B+D, /),
  3(4B+.15D"+3D, /)" ), AUX[1], AUX[3], AUX[5], AUX[7], AUX[9])
"END"

```

## INPUT:

```

+ 4 + 2 + 4 + 1
+30 +20 +45 +12
+20 +15 +36 +10
+35 +28 +70 +20

```

## RESULTS:

```

CALCULATED INVERSE:
+4 -2 +4 -1
-30 +20 -45 +12
+20 -15 +36 -10
-35 +28 -70 +20

```

## AUX ELEMENTS:

```

+1
+4
+.7000000000000000"+002
+.112528571428570"+003
+.1549999999999730"+003

```

SECTION: 3.1.1.1.1.4

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SUBSECTION: GSSINVERB.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" GSSINVERB(A, N, AUX); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE MATRIX, WHOSE INVERSE HAS TO BE CALCULATED;  
 EXIT: IF AUX[3] = N, THEN THE CALCULATED INVERSE MATRIX;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[0:11];  
 ENTRY:  
 AUX[0]: THE MACHINE PRECISION;  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 AUX[4]: A VALUE WHICH IS USED FOR CONTROLLING PIVOTING (SEE  
 GSSELM, SECTION 3.1.1.1.1.1);  
 AUX[5]: AN UPPER BOUND FOR THE RELATIVE PRECISION OF THE  
 GIVEN MATRIX ELEMENTS;

EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R  
 IS POSITIVE, ELSE AUX[1] = -1;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 AUX[3] < N THEN THE PROCESS IS TERMINATED AND NO  
 SOLUTION WILL HAVE BEEN CALCULATED;  
 AUX[5]: THE MODULUS OF AN ELEMENT WHICH IS OF MAXIMUM  
 ABSOLUTE VALUE FOR THE MATRIX GIVEN IN ARRAY A;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH (SEE GSSELM, SECTION  
 3.1.1.1.1.1);  
 AUX[9]: IF AUX[3] = N, THEN AUX[9] WILL EQUAL THE 1-NORM OF  
 THE INVERSE MATRIX, ELSE AUX[9] WILL BE UNDEFINED;  
 AUX[11]: IF AUX[3] = N THEN THE VALUE OF AUX[11] WILL BE A  
 ROUGH UPPER BOUND FOR THE RELATIVE ERROR IN THE  
 CALCULATED INVERSE MATRIX, ELSE AUX[11] WILL BE  
 BE UNDEFINED; IF NO USE CAN BE MADE OF THE FORMULA  
 FOR THE ERROR BOUND AS GIVEN IN SECTION  
 3.1.1.1.1.1 (SUBSECTION ERBELM), BECAUSE OF A  
 VERY BAD CONDITION OF THE MATRIX, THEN AUX[11] = -1.

PROCEDURES USED:

INV1 = CP34235,  
 GSSELM = CP34231,  
 ERBELM = CP34241.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: GSSINVERB DECLARES TWO AUXILIARY ARRAYS OF TYPE INTEGER AND ORDER N.

RUNNING TIME: PROPORTIONAL TO  $N ** 3$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

GSSINVERB USES GSSELM (SECTION 3.1.1.1.1.1) TO PERFORM THE TRIANGULAR DECOMPOSITION OF THE MATRIX, INV1 (THIS SECTION) TO CALCULATE THE INVERSE MATRIX AND ITS 1-NORM AND ERBELM (SECTION 3.1.1.1.1.1) TO CALCULATE AN UPPER BOUND FOR THE RELATIVE ERROR IN THE CALCULATED INVERSE; IF  $AUX[3] < N$ , THEN THE EFFECT OF GSSINVERB IS MERELY THAT OF GSSELM.

EXAMPLE OF USE:

THE FOLLOWING PROGRAM CALCULATES THE INVERSE OF THE INPUT MATRIX WITH AN UPPER BOUND FOR THE RELATIVE ERROR IN IT AND PRINTS THE RESULTS:

```
"BEGIN"
  "ARRAY" A[1:4, 1:4], AUX[0:11];
  "PROCEDURE" GSSINVERB(A, N, AUX); "CODE" 34244;
  "PROCEDURE" LIST(ITEM); "PROCEDURE" ITEM;
  "BEGIN" "INTEGER" I, J;
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
      "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO" ITEM(A[I,J])
  "END" LIST;
  "PROCEDURE" LAYOUT;
  FORMAT("("4(4B,4(B+ZDB),/),/)"");

  INLIST(70, LAYOUT, LIST); AUX[0]:= AUX[2]:= AUX[6]:= "-14";
  AUX[4]:= 8; GSSINVERB(A, 4, AUX);
  OUTPUT(71, ("(/, ("CALCULATED INVERSE:)",/)"");
  OUTLIST(71, LAYOUT, LIST);
  OUTPUT(71, ("4B("AUX ELEMENTS:)",/,2(4B+D,/),
  4(4B+.15D"+3D,/)"", AUX[1], AUX[3], AUX[5], AUX[7], AUX[9],
  AUX[11])
"END"
```

INPUT:

+ 4	+ 2	+ 4	+ 1
+30	+20	+45	+12
+20	+15	+36	+10
+35	+28	+70	+20

RESULTS:

CALCULATED INVERSE:

+4	-2	+4	-1
-30	+20	-45	+12
+20	-15	+36	-10
-35	+28	-70	+20

AUX ELEMENTS:

+1  
+4  
+,7000000000000000"+002  
+,112528571428570"+003  
+,154999999999730"+003  
+,222946341369190"-007

REFERENCES:

- [1] BUS, J. C. P.  
 LINEAR SYSTEMS WITH CALCULATION OF ERROR BOUNDS AND ITERATIVE  
 REFINEMENT (DUTCH).  
 MATHEMATICAL CENTRE, AMSTERDAM, LR 3. 4. 19 (1972).
- [2] DEKKER, T. J.  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 1.  
 MATHEMATICAL CENTRE, AMSTERDAM, TRACT 22 (1968).

## SOURCE TEXT(S):

```

"CODE" 34053;
  "PROCEDURE" INV(A, N, P); "VALUE" N; "INTEGER" N; "ARRAY" A;
  "INTEGER" "ARRAY" P;
  "BEGIN" "INTEGER" J, K, K1;
    "REAL" R;
    "ARRAY" V[1:N];
    "REAL" "PROCEDURE" MATMAT(L, U, I, J, A, B); "CODE" 34013;
    "PROCEDURE" ICHCOL(L, U, I, J, A); "CODE" 34031;
    "PROCEDURE" DUPCOLVEC(L, U, J, A, B); "CODE" 31034;
    "FOR" K:= N "STEP" = 1 "UNTIL" 1 "DO"
      "BEGIN" K1:= K + 1;
        "FOR" J:= N "STEP" = 1 "UNTIL" K1 "DO"
          "BEGIN" A[J,K1]:= V[J];
            V[J]:= - MATMAT(K1, N, K, J, A, A)
          "END";
          R:= A[K,K];
          "FOR" J:= N "STEP" = 1 "UNTIL" K1 "DO"
            "BEGIN" A[K,J]:= V[J];
              V[J]:= - MATMAT(K1, N, J, K, A, A) / R
            "END";
            V[K]:= (1 - MATMAT(K1, N, K, K, A, A)) / R
          "END";
        DUPCOLVEC(1, N, 1, A, V);
        "FOR" K:= N - 1 "STEP" = 1 "UNTIL" 1 "DO"
          "BEGIN" K1:= P[K]; "IF" K1 "≠" K "THEN"
            ICHCOL(1, N, K, K1, A)
          "END"
        "END" INV;
      "EOP"

"CODE" 34302;
  "PROCEDURE" DECINV(A, N, AUX); "VALUE" N; "INTEGER" N;
  "ARRAY" A, AUX;
  "BEGIN" "INTEGER" "ARRAY" P[1:N];
    "PROCEDURE" DEC(A, N, AUX, P); "CODE" 34300;
    "PROCEDURE" INV(A, N, P); "CODE" 34053;
    DEC(A, N, AUX, P); "IF" AUX[3] = N "THEN" INV(A, N, P)
  "END" DECINV;
  "EOP"

```

```

"CODE" 34235;
"REAL" "PROCEDURE" INV1(A, N, RI, CI, WITHNORM);
"VALUE" N, WITHNORM; "INTEGER" N; "BOOLEAN" WITHNORM;
"ARRAY" A; "INTEGER" "ARRAY" RI, CI;
"BEGIN" "INTEGER" L, K, K1;
  "REAL" AID, NRMINV;
  "PROCEDURE" ICHROW(L, U, I, J, A); "CODE" 34032;
  "PROCEDURE" INV(A, N, P); "CODE" 34053;
  INV(A, N, RI); NRMINV:= 0; "IF" WITHNORM "THEN"
  "FOR" L:= 1 "STEP" 1 "UNTIL" N "DO"
  NRMINV:= NRMINV + ABS(A[L,N]);
  "FOR" K:= N - 1 "STEP" - 1 "UNTIL" 1 "DO"
  "BEGIN" "IF" WITHNORM "THEN"
    "BEGIN" AID:= 0;
    "FOR" L:= 1 "STEP" 1 "UNTIL" N "DO"
    AID:= AID + ABS(A[L,K]);
    "IF" NRMINV < AID "THEN" NRMINV:= AID
  "END";
  K1:= CI[K]; "IF" K1 # K "THEN" ICHROW(1, N, K, K1, A)
"END";
  INV1:= NRMINV
"END" INV1;
"EOP"

"CODE" 34236;
"PROCEDURE" GSSINV(A, N, AUX); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX;
"BEGIN" "INTEGER" "ARRAY" RI, CI[1:N];
  "PROCEDURE" GSSELM(A, N, AUX, RI, CI); "CODE" 34231;
  "REAL" "PROCEDURE" INV1(A, N, RI, CI, WITHNORM); "CODE" 34235;
  GSSELM(A, N, AUX, RI, CI);
  "IF" AUX[3] = N "THEN" AUX[9]:= INV1(A, N, RI, CI, "TRUE")
"END" GSSINV;
"EOP"

"CODE" 34244;
"PROCEDURE" GSSINVERB(A, N, AUX); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX;
"BEGIN" "INTEGER" "ARRAY" RI, CI[1:N];
  "PROCEDURE" GSSELM(A, N, AUX, RI, CI); "CODE" 34231;
  "REAL" "PROCEDURE" INV1(A, N, RI, CI, WITHNORM); "CODE" 34235;
  "PROCEDURE" ERBELM(N, AUX, NRMINV); "CODE" 34241;
  GSSELM(A, N, AUX, RI, CI);
  "IF" AUX[3] = N "THEN"
  ERBELM(N, AUX, INV1(A, N, RI, CI, "TRUE"))
"END" GSSINVERB;
"EOP"

```



SECTION: 3.1,1.1.1.1.5

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BRIEF DESCRIPTION:

THIS SECTION CONTAINS FOUR PROCEDURES FOR CALCULATING AN ITERATIVELY IMPROVED SOLUTION OF A SYSTEM OF LINEAR EQUATIONS; ITISOL SOLVES A LINEAR SYSTEM WHOSE MATRIX HAS BEEN TRIANGULARLY DECOMPOSED BY GSSELM OR GSSERB, THIS SOLUTION IS IMPROVED ITERATIVELY; GSSITISOL SOLVES A LINEAR SYSTEM AND THIS SOLUTION IS IMPROVED ITERATIVELY; ITISOLERB SOLVES A LINEAR SYSTEM WHOSE MATRIX HAS BEEN TRIANGULARLY DECOMPOSED BY GSSNRI, THIS SOLUTION IS IMPROVED ITERATIVELY, MOREOVER A REALISTIC UPPERBOUND FOR THE RELATIVE ERROR IN THE SOLUTION IS CALCULATED. GSSITISOLERB SOLVES A LINEAR SYSTEM, THIS SOLUTION IS IMPROVED ITERATIVELY AND A REALISTIC UPPERBOUND FOR THE RELATIVE ERROR IN THE SOLUTION IS CALCULATED;

KEYWORDS:

ALGEBRAIC EQUATIONS,  
 LINEAR SYSTEMS,  
 ITERATIVE REFINEMENT,

SUBSECTION: ITISOL

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" ITISOL(A, LU, N, AUX, RI, CI, B); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, LU, AUX, B; "INTEGER" "ARRAY" RI, CI;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE MATRIX OF THE LINEAR SYSTEM;

LU: <ARRAY IDENTIFIER>;  
 "ARRAY" LU[1:N, 1:N];  
 ENTRY: THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX GIVEN  
 IN A, AS DELIVERED BY GSSELM (SECTION 3.1.1.1.1.1);

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[10:13];  
 ENTRY:  
 AUX[10]: A RELATIVE TOLERANCE FOR THE SOLUTION VECTOR; IF  
 THE 1-NORM OF THE VECTOR OF CORRECTIONS TO THE  
 SOLUTION, DIVIDED BY THE 1-NORM OF THE CALCULATED  
 SOLUTION, IS SMALLER THAN AUX[10], THEN THE PROCESS  
 WILL STOP; THE USER SHOULD NOT CHOOSE THE VALUE OF  
 AUX[10] SMALLER THAN THE RELATIVE PRECISION OF THE  
 ELEMENTS OF THE MATRIX AND THE RIGHT-HAND SIDE OF  
 THE LINEAR SYSTEM;  
 AUX[12]: THE MAXIMUM NUMBER OF ITERATIONS ALLOWED FOR THE  
 REFINEMENT OF THE SOLUTION; IF THE NUMBER OF  
 ITERATIONS EXCEEDS THE VALUE OF AUX[12], THEN THE  
 PROCESS WILL BE BROKEN OFF; USUALLY AUX[12] = 5  
 WILL GIVE GOOD RESULTS;

EXIT:  
 AUX[11]: THE 1-NORM OF THE VECTOR OF CORRECTIONS TO THE  
 SOLUTION IN THE LAST ITERATION STEP, DIVIDED BY THE  
 1-NORM OF THE CALCULATED SOLUTION;  
 IF AUX[11] > AUX[10], THEN THE PROCESS HAS BEEN  
 TERMINATED, BECAUSE THE NUMBER OF ITERATIONS  
 EXCEEDED THE VALUE GIVEN IN AUX[12];  
 AUX[13]: THE 1-NORM OF THE RESIDUAL VECTOR (SEE METHOD AND  
 PERFORMANCE;

RI: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" RI[1:N];  
 ENTRY: THE PIVOTAL ROW INDICES, AS PRODUCED BY GSSELM;

CI: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" CI[1:N];  
 ENTRY: THE PIVOTAL COLUMN INDICES, AS PRODUCED BY GSSELM;

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: THE SOLUTION OF THE LINEAR SYSTEM.

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## PROCEDURES USED:

SOLELM = CP34051,  
 INIVEC = CP31010,  
 DUPVEC = CP31030,  
 LNGMATVEC = CP34411.

## REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: ITISOL DECLARES TWO AUXILIARY ARRAYS OF TYPE REAL AND ORDER N.

RUNNING TIME: THE NUMBER OF ARITHMETICAL OPERATIONS IN EACH ITERATION STEP IS PROPORTIONAL TO  $N^{**}2$ .

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

ITISOL SHOULD BE CALLED AFTER GSSELM OR GSSERB (SECTION 3.1.1.1.1.1) AND SOLVES THE LINEAR SYSTEM WITH A MATRIX, AS GIVEN IN ARRAY A AND A RIGHT-HAND SIDE AS GIVEN IN ARRAY B; ONCE A SOLUTION IS CALCULATED WITH SOLELM (SECTION 3.1.1.1.1.3), THIS SOLUTION WILL BE REFINED ITERATIVELY UNTIL THE CALCULATED RELATIVE CORRECTION TO THIS SOLUTION WILL BE LESS THAN A PRESCRIBED VALUE (SEE AUX[10]);

EACH ITERATION OF THE REFINEMENT PROCESS CONSISTS OF THE FOLLOWING THREE STEPS (SEE [1], [2], [3]):

- 1 CALCULATE, IN DOUBLE PRECISION, THE RESIDUAL VECTOR R, DEFINED BY:  

$$R = AX - B,$$
 WHERE X DENOTES THE SOLUTION, OBTAINED IN THE PREVIOUS ITERATION, B THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM, GIVEN IN B[1:N], AND A THE MATRIX GIVEN IN A[1:N, 1:N];
- 2 CALCULATE THE SOLUTION C, SAY, OF THE LINEAR SYSTEM:  $AC = R$ , WITH THE AID OF THE TRIANGULARLY DECOMPOSED MATRIX AS GIVEN IN LU[1:N, 1:N];
- 3 CALCULATE THE NEW SOLUTION:  $XNEW = X - C$ ;

IF THE PRECISION ASKED FOR IS PROPERLY CHOSEN (SEE AUX[10]) AND THE CONDITION OF THE MATRIX IS NOT TOO BAD, THEN THE PRECISION OF THE CALCULATED SOLUTION WILL BE OF THE ORDER OF THE PRECISION ASKED FOR IN AUX[10]; HOWEVER, IF THE CONDITION OF THE MATRIX IS VERY BAD, THEN THIS PROCESS WILL POSSIBLY NOT CONVERGE OR, IN EXCEPTIONAL CASES, CONVERGE TO A USELESS RESULT; IF THE USER WANTS TO MAKE CERTAIN ABOUT THE PRECISION OF THE CALCULATED SOLUTION, THEN HE HAS TO USE ITISOLERB (THIS SECTION), WHICH NEEDS THE CALCULATION (OF ORDER  $N^{**}3$ ) OF THE INVERSE MATRIX TO GET AN UPPER BOUND FOR THE CONDITION NUMBER AND WHICH GIVES A REALISTIC UPPER BOUND FOR THE RELATIVE ERROR IN THE CALCULATED SOLUTION;

ITISOL LEAVES A, LU, RI AND CI UNALTERED, SO AFTER ONE CALL OF GSSELM SEVERAL CALLS OF ITISOL MAY FOLLOW TO CALCULATE THE SOLUTION OF SEVERAL LINEAR SYSTEMS WITH THE SAME MATRIX BUT DIFFERENT RIGHT-HAND SIDES.

EXAMPLE OF USE: SEE GSSITISOL (THIS SECTION).

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SUBSECTION: GSSITISOL .

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" GSSITISOL(A, N, AUX, B); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE N-TH ORDER MATRIX;  
 EXIT: THE CALCULATED LOWER-TRIANGULAR MATRIX AND UNIT  
 UPPERTRIANGULAR MATRIX WITH ITS UNIT DIAGONAL OMITTED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[1:13];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 AUX[4]: A VALUE WHICH IS USED FOR CONTROLLING PIVOTING (SEE  
 GSSELM, SECTION 3.1.1.1.1.1);  
 AUX[10]: A RELATIVE TOLERANCE FOR THE SOLUTION VECTOR; IF  
 THE 1-NORM OF THE VECTOR OF CORRECTIONS TO THE  
 SOLUTION, DIVIDED BY THE 1-NORM OF THE CALCULATED  
 SOLUTION, IS SMALLER THAN AUX[10], THEN THE PROCESS  
 WILL STOP; THE USER SHOULD NOT CHOOSE THE VALUE OF  
 AUX[10] SMALLER THAN THE RELATIVE PRECISION OF THE  
 ELEMENTS OF THE MATRIX AND THE RIGHT-HAND SIDE OF  
 THE LINEAR SYSTEM;  
 AUX[12]: THE MAXIMUM NUMBER OF ITERATIONS ALLOWED FOR THE  
 REFINEMENT OF THE SOLUTION; IF THE NUMBER OF  
 ITERATIONS EXCEEDS THE VALUE OF AUX[12], THEN THE  
 PROCESS WILL BE BROKEN OFF; USUALLY AUX[12] = 5  
 WILL GIVE GOOD RESULTS;

EXIT:  
 AUX[1]: IF R IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER R  
 IS POSITIVE, ELSE AUX[1] = -1;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 AUX[3] < N THEN THE PROCESS IS TERMINATED AND NO  
 SOLUTION WILL HAVE BEEN CALCULATED;  
 AUX[5]: THE MODULUS OF AN ELEMENT WHICH IS OF MAXIMUM  
 ABSOLUTE VALUE FOR THE MATRIX GIVEN IN ARRAY A;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH (SEE GSSELM, SECTION  
 3.1.1.1.1.1);

AUX[11]: IF AUX[3] < N, THEN AUX[11] WILL BE UNDEFINED, ELSE AUX[11] EQUALS THE 1-NORM OF THE VECTOR OF CORRECTIONS TO THE SOLUTION IN THE LAST STEP, DIVIDED BY THE 1-NORM OF THE CALCULATED SOLUTION; IF AUX[11] > AUX[10], THEN THE PROCESS HAS BEEN TERMINATED, BECAUSE THE NUMBER OF ITERATIONS EXCEEDED THE VALUE GIVEN IN AUX[12];

AUX[13]: IF AUX[3] = N, THEN THE VALUE OF AUX[13] WILL EQUAL THE 1-NORM OF THE RESIDUAL VECTOR (SEE ITISOL IN THIS SECTION), ELSE AUX[13] WILL BE UNDEFINED;

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];

ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;

EXIT: IF AUX[3] = N, THEN THE CALCULATED SOLUTION OF THE LINEAR SYSTEM IS OVERWRITTEN ON B, ELSE B REMAINS UNALTERED.

PROCEDURES USED:

DUPMAT = CP34035,  
 GSSELM = CP34231,  
 ITISOL = CP34250.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: GSSITISOL DECLARES ONE AUXILIARY ARRAY OF TYPE REAL AND ORDER  $N ** 2$  AND TWO OF TYPE INTEGER AND ORDER  $N$ .

RUNNING TIME: PROPORTIONAL TO  $N ** 3$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

GSSITISOL USES GSSELM (SECTION 3.1.1.1.1.1) TO PERFORM A TRIANGULAR DECOMPOSITION OF THE MATRIX AND ITISOL (THIS SECTION) TO CALCULATE AN ITERATIVELY REFINED SOLUTION OF THE GIVEN LINEAR SYSTEM; IF AUX[3] < N, THEN THE EFFECT OF GSSITISOL IS MERELY THAT OF GSSELM; IF THE CONDITION OF THE MATRIX IS VERY BAD, THEN, IN EXCEPTIONAL CASES, THE CALCULATED SOLUTION MAY BE USELESS (SEE ITISOL IN THIS SECTION).

EXAMPLE OF USE:

LET A BE THE FOURTH ORDER SEGMENT OF THE HILBERT MATRIX, MULTIPLIED WITH 840 TO GET INTEGER ELEMENTS, AND B THE THIRD COLUMN OF A, THEN THE SOLUTION OF THE LINEAR SYSTEM  $AX = B$  IS GIVEN BY THE THIRD UNIT VECTOR AND MAY BE CALCULATED BY THE FOLLOWING PROGRAM:

```
"BEGIN" "INTEGER" I, J;
  "ARRAY" A[1:4, 1:4], B[1:4], AUX[1:13];
  "PROCEDURE" GSSITISOL(A, N, AUX, B); "CODE" 34251;
  "PROCEDURE" LIST(ITEM); "PROCEDURE" ITEM;
  "BEGIN" "INTEGER" I;
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO" ITEM(B[I]);
    "FOR" I:= 1 "STEP" 2 "UNTIL" 7 "DO" ITEM(AUX[I]);
    ITEM(AUX[11]); ITEM(AUX[13])
  "END" LIST;
  "PROCEDURE" LAYOUT;
  FORMAT("(*, ("SOLUTION:")"B+,15D"+3D,/,3(10B+,15D"+3D,/,
  ("SIGN(DET) = ")"+D,/,("NUMBER OF ELIMINATIONSTEPS = ")"
  +D,/,("MAX(ABS(A[I,J]))= ")"+,15D"+3D,/,
  ("UPPER BOUND GROWTH: ")"+,15D"+3D,/,
  ("NORM LAST CORRECTION VECTOR: ")"+,15D"+3D,/,
  ("NORM RESIDUAL VECTOR: ")"+,15D"+3D")");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    A[I,J]:= 840 // (I + J - 1); B[I]:= A[I,3]
  "END";
  AUX[2]:= "-14; AUX[4]:= 8; AUX[10]:= "-14; AUX[12]:= 5;
  GSSITISOL(A, 4, AUX, B);
  OUTLIST(71, LAYOUT, LIST)
"END"
```

RESULTS:

```
SOLUTION: +.0000000000000000"+000
           +.0000000000000000"+000
           +.1000000000000000"+001
           +.0000000000000000"+000
SIGN(DET) = +1
NUMBER OF ELIMINATIONSTEPS = +4
MAX(ABS(A[I,J]))= +.8400000000000000"+003
UPPER BOUND GROWTH: +.1340800000000000"+004
NORM LAST CORRECTION VECTOR: +.0000000000000000"+000
NORM RESIDUAL VECTOR: +.0000000000000000"+000
```

SECTION: 3.1.1.1.1.1.5

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SUBSECTION: ITISOLERB.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:

"PROCEDURE" ITISOLERB(A, LU, N, AUX, RI, CI, B); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, LU, AUX, B; "INTEGER" "ARRAY" RI, CI;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" [1:N,1:N];  
 ENTRY: THE MATRIX OF THE LINEAR SYSTEM;

LU: <ARRAY IDENTIFIER>;  
 "ARRAY" LU[1:N,1:N];  
 ENTRY: THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX GIVEN  
 IN A AS DELIVERED BY GSSNRI (SECTION 3.1.1.1.1.1.1);

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[0:13];  
 ENTRY:  
 AUX[0]: THE MACHINE PRECISION;  
 AUX[5]: THE MODULUS OF AN ELEMENT, WHICH IS OF MAXIMUM  
 ABSOLUTE VALUE FOR THE MATRIX OF THE LINEAR SYSTEM;  
 THIS VALUE IS DELIVERED BY GSSNRI (SECTION  
 3.1.1.1.1.1.1) IN AUX[5];  
 AUX[6]: AN UPPER BOUND FOR THE RELATIVE ERROR IN THE  
 ELEMENTS OF THE MATRIX OF THE LINEAR SYSTEM;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH DURING GAUSSIAN  
 ELIMINATION; THIS VALUE IS DELIVERED BY GSSNRI IN  
 AUX[7];  
 AUX[8]: AN UPPER BOUND FOR THE RELATIVE ERROR IN THE  
 ELEMENTS OF THE RIGHT-HAND SIDE OF THE LINEAR  
 SYSTEM;  
 AUX[9]: THE 1-NORM OF THE INVERSE MATRIX; THIS VALUE IS  
 DELIVERED BY GSSNRI IN AUX[9];  
 AUX[10]: A RELATIVE TOLERANCE FOR THE SOLUTION VECTOR; IF  
 THE 1-NORM OF THE VECTOR OF CORRECTIONS TO THE  
 SOLUTION, DIVIDED BY THE 1-NORM OF THE CALCULATED  
 SOLUTION, IS SMALLER THAN AUX[10], THEN THE PROCESS  
 WILL STOP; THE USER SHOULD NOT CHOOSE THE VALUE OF  
 AUX[10] SMALLER THAN THE RELATIVE PRECISION OF THE  
 ELEMENTS OF THE MATRIX AND THE RIGHT-HAND SIDE OF  
 THE LINEAR SYSTEM, GIVEN IN AUX[6] AND AUX[8];  
 AUX[12]: THE MAXIMUM NUMBER OF ITERATIONS ALLOWED FOR THE  
 REFINEMENT OF THE SOLUTION; IF THE NUMBER OF  
 ITERATIONS EXCEEDS THE VALUE OF AUX[12], THEN THE  
 PROCESS WILL BE BROKEN OFF; USUALLY AUX[12] = 5  
 WILL GIVE GOOD RESULTS;

EXIT:  
 AUX[11]: A REALISTIC UPPERBOUND FOR THE RELATIVE ERROR IN  
 THE CALCULATED SOLUTION; HOWEVER, IF NO USE CAN BE  
 MADE OF THE ERROR-FORMULA, THEN AUX[11] := -1;  
 AUX[13]: THE 1-NORM OF THE RESIDUAL VECTOR (SEE METHOD AND  
 PERFORMANCE);  
 RI: <ARRAY IDENTIFIER>;  
 "INTEGER""ARRAY" RI[1:N];  
 ENTRY: THE PIVOTAL ROW INDICES, AS PRODUCED BY GSSNRI;  
 CI: <ARRAY IDENTIFIER>;  
 "INTEGER""ARRAY" CI[1:N];  
 EXIT: THE PIVOTAL COLUMN INDICES, AS PRODUCED BY GSSNRI;  
 B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: THE SOLUTION OF THE LINEAR SYSTEM.

## PROCEDURES USED:

ITISOL = CP34250.

RUNNING TIME: THE NUMBER OF ARITHMETICAL OPERATIONS IN EACH ITERATION  
 STEP OF THE REFINEMENT PROCESS IS PROPORTIONAL TO  $N^{**}2$ .

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

ITISOLERB SHOULD BE CALLED AFTER GSSNRI (SECTION 3.1.1.1.1.1.1),  
 WHICH DELIVERS THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX AND  
 THE PROPER VALUES FOR THE ODD ELEMENTS OF ARRAY AUX; ITISOLERB  
 CALCULATES, WITH THE USE OF ITISOL (THIS SECTION), AN ITERATIVELY  
 IMPROVED SOLUTION OF THE LINEAR SYSTEM WITH A MATRIX AS GIVEN IN  
 ARRAY A AND A RIGHT-HAND SIDE AS GIVEN IN B; MOREOVER, ITISOLERB  
 CALCULATES A REALISTIC UPPER BOUND FOR THE RELATIVE ERROR IN THE  
 CALCULATED SOLUTION; THIS UPPER BOUND IS CALCULATED WITH THE  
 FOLLOWING FORMULA (SEE [1],[2]):

$$\text{NORM}(DX) / \text{NORM}(X) \leq P / (1 - P),$$
 WHEREBY:  $P = (\text{NORM}(R) / \text{NORM}(X) + \text{NORM}(DB) / \text{NORM}(X) + \text{NORM}(DA) )$   

$$* \text{NORM}(C) / (1 - Q * \text{NORM}(C) )$$
 FOR Q SEE SECTION 3.1.1.1.1.1.1 (SUBSECTION ERBELM),  
 R IS THE RESIDUAL VECTOR (SEE ITISOL IN THIS SECTION),  
 X IS THE CALCULATED SOLUTION,  
 DB IS THE UPPER BOUND FOR THE RELATIVE ERROR IN THE RIGHT-HAND  
 SIDE,  
 DA IS THE UPPER BOUND FOR THE RELATIVE ERROR IN THE MATRIX,  
 C IS THE CALCULATED INVERSE MATRIX,  
 AND THE 1-NORM OF A VECTOR OR A MATRIX IS DENOTED BY: NORM(.)



IF  $1 - P < \text{AUX}[0]$ , THEN THE VALUE =1 IS DELIVERED IN  $\text{AUX}[11]$ ;  
 ITISOLERB LEAVES A, LU, RI AND CI UNALTERED, SO AFTER ONE CALL OF  
 GSSNRI SEVERAL CALLS OF ITISOLERB MAY FOLLOW, TO CALCULATE THE  
 SOLUTION OF SEVERAL LINEAR SYSTEMS WITH THE SAME MATRIX BUT  
 DIFFERENT RIGHT-HAND SIDES,

EXAMPLE OF USE: SEE GSSITISOLERB (THIS SECTION).

SUBSECTION: GSSITISOLERB.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" GSSITISOLERB(A, N, AUX, B); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

- A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE N-TH ORDER MATRIX;  
 EXIT: THE CALCULATED LOWER-TRIANGULAR MATRIX AND UNIT  
 UPPER-TRIANGULAR MATRIX WITH ITS UNIT DIAGONAL OMITTED;
- N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;
- AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[0:13];  
 ENTRY:  
 AUX[0]: THE MACHINE PRECISION;  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS; HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 AUX[4]: A VALUE WHICH IS USED FOR CONTROLLING PIVOTING (SEE  
 GSSELM, SECTION 3.1.1.1.1.1);  
 AUX[6]: AN UPPER BOUND FOR THE RELATIVE ERROR IN THE MATRIX  
 ELEMENTS OF THE LINEAR SYSTEM;  
 AUX[8]: AN UPPER BOUND FOR THE RELATIVE ERROR IN THE  
 ELEMENTS OF THE RIGHT-HAND SIDE;  
 AUX[10]: A RELATIVE TOLERANCE FOR THE SOLUTION VECTOR; IF  
 THE 1-NORM OF THE VECTOR OF CORRECTIONS TO THE  
 SOLUTION, DIVIDED BY THE 1-NORM OF THE CALCULATED  
 SOLUTION, IS SMALLER THAN AUX[10], THEN THE PROCESS  
 WILL STOP; THE USER SHOULD NOT CHOOSE THE VALUE OF  
 AUX[10] SMALLER THAN THE RELATIVE PRECISION OF THE  
 ELEMENTS OF THE MATRIX AND THE RIGHT-HAND SIDE OF  
 THE LINEAR SYSTEM;  
 AUX[12]: THE MAXIMUM NUMBER OF ITERATIONS ALLOWED FOR THE  
 REFINEMENT OF THE SOLUTION; IF THE NUMBER OF  
 ITERATIONS EXCEEDS THE VALUE OF AUX[12], THEN THE  
 PROCESS WILL BE BROKEN OFF; USUALLY  $\text{AUX}[12] = 5$   
 WILL GIVE GOOD RESULTS;

EXIT:  
 AUX[1]: IF  $R$  IS THE NUMBER OF ELIMINATION STEPS PERFORMED  
 (SEE AUX[3]), THEN AUX[1] EQUALS 1 IF THE  
 DETERMINANT OF THE PRINCIPAL SUBMATRIX OF ORDER  $R$   
 IS POSITIVE, ELSE  $AUX[1] = -1$ ;  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED; IF  
 $AUX[3] < N$  THEN THE PROCESS IS TERMINATED AND NO  
 SOLUTION WILL HAVE BEEN CALCULATED;  
 AUX[5]: THE MODULUS OF AN ELEMENT WHICH IS OF MAXIMUM  
 ABSOLUTE VALUE FOR THE MATRIX GIVEN IN ARRAY A;  
 AUX[7]: AN UPPER BOUND FOR THE GROWTH (SEE GSSELM, SECTION  
 3.1.1.1.1.1);  
 AUX[9]: IF  $AUX[3] = N$  THEN AUX[9] EQUALS THE 1-NORM OF THE  
 CALCULATED INVERSE MATRIX, ELSE AUX[9] WILL BE  
 UNDEFINED;  
 AUX[11]: IF  $AUX[3] < N$ , THEN AUX[11] WILL BE UNDEFINED,  
 ELSE THE VALUE OF AUX[11] EQUALS A REALISTIC UPPER  
 BOUND FOR THE RELATIVE ERROR IN THE CALCULATED  
 SOLUTION; HOWEVER, IF NO USE CAN BE MADE OF THE  
 ERROR FORMULA (SEE ITISOLERB IN THIS SECTION), THEN  
 $AUX[11] := -1$ ;  
 AUX[13]: IF  $AUX[3] = N$ , THEN AUX[13] EQUALS THE 1-NORM OF  
 THE RESIDUAL VECTOR (SEE ITISOL IN THIS SECTION),  
 ELSE AUX[13] WILL BE UNDEFINED;  
 B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: IF  $AUX[3] = N$ , THEN THE CALCULATED SOLUTION OF THE  
 LINEAR SYSTEM IS OVERWRITTEN ON B, ELSE B REMAINS  
 UNALTERED.

## PROCEDURES USED:

DUPMAT = CP34035,  
 GSSNRI = CP34252,  
 ITISOLERB = CP34253.

## REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: GSSITISOLERB DECLARES ONE AUXILIARY ARRAY  
 OF TYPE REAL AND ORDER  $N ** 2$  AND TWO OF  
 TYPE INTEGER AND ORDER  $N$ .

RUNNING TIME: PROPORTIONAL TO  $N ** 3$ ,  
 LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

GSSITISOLERB USES GSSNRI (SECTION 3.1.1.1.1.1) TO PERFORM A  
 TRIANGULAR DECOMPOSITION OF THE MATRIX AND ITISOLERB (THIS SECTION)  
 TO CALCULATE AN ITERATIVELY REFINED SOLUTION OF THE GIVEN LINEAR  
 SYSTEM AND A REALISTIC UPPER BOUND FOR THE RELATIVE ERROR IN THIS  
 SOLUTION; IF  $AUX[3] < N$ , THEN THE EFFECT OF GSSITISOLERB IS MERELY  
 THAT OF GSSELM (SECTION 3.1.1.1.1.1).

EXAMPLE OF USE:

LET A BE THE FOURTH ORDER SEGMENT OF THE HILBERT MATRIX, MULTIPLIED WITH 840 TO GET INTEGER ELEMENTS, AND B THE THIRD COLUMN OF A, THEN THE SOLUTION OF THE LINEAR SYSTEM  $AX = B$  IS GIVEN BY THE THIRD UNIT VECTOR AND THIS SOLUTION, AS WELL AS A REALISTIC UPPER BOUND FOR THE RELATIVE ERROR IN IT, MAY BE CALCULATED BY THE FOLLOWING PROGRAM:

```
"BEGIN" "INTEGER" I, J;
  "ARRAY" A[1:4, 1:4], B[1:4], AUX[0:13];
  "PROCEDURE" GSSITISOLERB(A, N, AUX, B); "CODE" 34254;
  "PROCEDURE" LIST(ITEM); "PROCEDURE" ITEM;
  "BEGIN" "INTEGER" I;
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO" ITEM(B[I]);
    "FOR" I:= 1 "STEP" 2 "UNTIL" 13 "DO" ITEM(AUX[I])
  "END" LIST;
  "PROCEDURE" LAYOUT;
  FORMAT("(*, "("SOLUTION:"")B+,15D"+3D,/,3(10B+,15D"+3D,/,),
  "("SIGN(DET) = ")" +D,/, "("NUMBER OF ELIMINATIONSTEPS = ")"
  +D,/, "("MAX(ABS(A[I,J]))= ")" +.15D"+3D,/,
  "("UPPER BOUND GROWTH: ")" +.15D"+3D,/,
  "("NORM CALCULATED INVERSE MATRIX: ")" +.15D"+3D,/,
  "("UPPER BOUND FOR THE RELATIVE ERROR: ")" +.15D"+3D,/,
  "("NORM RESIDUAL VECTOR: ")" +.15D"+3D")");

  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    A[I,J]:= 840 // (I + J - 1); B[I]:= A[I,3]
  "END";
  AUX[0]:= AUX[2]:= "-14; AUX[4]:= 8; AUX[6]:= AUX[8]:= 0;
  AUX[10]:= "-14; AUX[12]:= 5;
  GSSITISOLERB(A, 4, AUX, B);
  OUTLIST(71, LAYOUT, LIST)
"END"
```

RESULTS:

```
SOLUTION: +.0000000000000000"+000
          +.0000000000000000"+000
          +.1000000000000000"+001
          +.0000000000000000"+000

SIGN(DET) = +1
NUMBER OF ELIMINATIONSTEPS = +4
MAX(ABS(A[I,J]))= +.8400000000000000"+003
UPPER BOUND GROWTH: +.1340800000000000"+004
NORM CALCULATED INVERSE MATRIX: +.162142857143540"+002
UPPER BOUND FOR THE RELATIVE ERROR: +.0000000000000000"+000
NORM RESIDUAL VECTOR: +.0000000000000000"+000
```

## REFERENCES:

- [1] BUS, J. C. P.  
 LINEAR SYSTEMS WITH CALCULATION OF ERROR BOUNDS AND ITERATIVE  
 REFINEMENT (DUTCH).  
 MATHEMATICAL CENTRE, AMSTERDAM, LR 3.4.19, (1972).
- [2] DEKKER, T. J.  
 NUMERICAL ALGEBRA (DUTCH).  
 MATHEMATICAL CENTRE, AMSTERDAM, SYLLABUS 12, (1971).
- [3] WILKINSON, J. H.  
 THE ALGEBRAIC EIGENVALUE PROBLEM,  
 OXFORD (1965).

## SOURCE TEXT(S):

```

"CODE" 34250;
"PROCEDURE" ITISOL(A, LU, N, AUX, RI, CI, B); "VALUE" N;
"INTEGER" N;
"ARRAY" A, LU, AUX, B; "INTEGER" "ARRAY" RI, CI;
"BEGIN" "INTEGER" I, ITER, MAXITER;
  "REAL" MAXERX, ERX, NRMRES, NRMSOL, R, RR;
  "ARRAY" RES, SOL[1:N];
  "PROCEDURE" SOLELM(A, N, RI, CI, B); "CODE" 34061;
  "PROCEDURE" INIVEC(L, U, A, X); "CODE" 31010;
  "PROCEDURE" DUPVEC(L, U, SHIFT, A, B); "CODE" 31030;
  "PROCEDURE" LNGMATVEC(A, B, C, D, E, F, G, H, I);
  "CODE" 34411;
  MAXERX := ERX := AUX[10]; MAXITER := AUX[12];
  INIVEC(1, N, SOL, 0); DUPVEC(1, N, 0, RES, B);
  "FOR" ITER := 1, ITER + 1 "WHILE" ITER <= MAXITER &
  MAXERX < ERX "DO"
  "BEGIN" SOLELM(LU, N, RI, CI, RES); ERX := NRMSOL := NRMRES := 0;
    "FOR" I := 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" R := RES[I]; ERX := ERX + ABS(R); RR := SOL[I] + R;
        SOL[I] := RR; NRMSOL := NRMSOL + ABS(RR)
      "END";
      ERX := ERX / NRMSOL;
      "FOR" I := 1 "STEP" 1 "UNTIL" N "DO"
        "BEGIN" LNGMATVEC(1, N, I, A, SOL, - B[I], 0, R, RR);
          R := - (R + RR); RES[I] := R; NRMRES := NRMRES + ABS(R)
        "END"
    "END" ITERATION;
  DUPVEC(1, N, 0, B, SOL);
  AUX[11] := ERX; AUX[13] := NRMRES
"END" ITISOL;
"EOP"

```

```

"CODE" 34251;
"PROCEDURE" GSSITISOL(A, N, AUX, B); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX, B;
"BEGIN" "INTEGER" I, J;
"ARRAY" AA[1:N,1:N];
"INTEGER" "ARRAY" RI, CI[1:N];
"PROCEDURE" GSSELM(A, N, AUX, RI, CI); "CODE" 34231;
"PROCEDURE" ITISOL(A, LU, N, AUX, RI, CI, B); "CODE" 34250;
"PROCEDURE" DUPMAT(L, U, I, J, A, B); "CODE" 31035;
DUPMAT(1, N, 1, N, AA, A);
GSSELM(A, N, AUX, RI, CI);
"IF" AUX[3] = N "THEN" ITISOL(AA, A, N, AUX, RI, CI, B)
"END" GSSITISOL;
"EOP"

"CODE" 34253;
"PROCEDURE" ITISOLERB(A, LU, N, AUX, RI, CI, B); "VALUE" N;
"INTEGER" N;
"ARRAY" A, LU, AUX, B; "INTEGER" "ARRAY" RI, CI;
"BEGIN" "INTEGER" I;
"REAL" NRMSOL, NRMINV, NRMB, ALFA, TOLA, EPS;
"PROCEDURE" ITISOL(A, LU, N, AUX, RI, CI, B); "CODE" 34250;
EPS:= AUX[10];
NRMINV:= AUX[9]; TOLA:= AUX[5] * AUX[6]; NRMB:= NRMSOL:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO" NRMB:= NRMB + ABS(B[I]);
ITISOL(A, LU, N, AUX, RI, CI, B);
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
NRMSOL:= NRMSOL + ABS(B[I]);
ALFA:= 1 - (1.06 * EPS * AUX[7] * (.75 * N + 4.5) * N ** 2
+ TOLA) * NRMINV;
"IF" ALFA < EPS "THEN" AUX[11]:= - 1 "ELSE"
"BEGIN" ALFA:= ((AUX[13] + AUX[8] * NRMB) / NRMSOL + TOLA) *
NRMINV / ALFA;
AUX[11]:= "IF" 1 - ALFA < EPS "THEN" = 1 "ELSE"
ALFA / (1 - ALFA)
"END"
"END" ITISOLERB;
"EOP"

"CODE" 34254;
"PROCEDURE" GSSITISOLERB(A, N, AUX, B); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX, B;
"BEGIN" "INTEGER" I, J;
"ARRAY" AA[1:N,1:N];
"INTEGER" "ARRAY" RI, CI[1:N];
"PROCEDURE" GSSNRI(A, N, AUX, RI, CI); "CODE" 34252;
"PROCEDURE" ITISOLERB(A, LU, N, AUX, RI, CI, B); "CODE" 34253;
"PROCEDURE" DUPMAT(L, U, I, J, A, B); "CODE" 31035;
DUPMAT(1, N, 1, N, AA, A);
GSSNRI(A, N, AUX, RI, CI);
"IF" AUX[3] = N "THEN" ITISOLERB(AA, A, N, AUX, RI, CI, B)
"END" GSSITISOLERB;
"EOP"
    
```

SECTION: 3.1.1.1.1.2.1

(MAY 1974)

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RECEIVED: 731015.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS TWO PROCEDURES:

A) CHLDEC2 CALCULATES THE CHOLESKY DECOMPOSITION OF A POSITIVE DEFINITE SYMMETRIC MATRIX WHOSE UPPER TRIANGLE IS GIVEN IN A TWO-DIMENSIONAL ARRAY;

B) CHLDEC1 CALCULATES THE CHOLESKY DECOMPOSITION OF A POSITIVE DEFINITE SYMMETRIC MATRIX WHOSE UPPER TRIANGLE IS GIVEN COLUMNWISE IN A ONE-DIMENSIONAL ARRAY.

KEYWORDS:

LINEAR EQUATIONS,  
POSITIVE DEFINITE SYMMETRIC MATRIX,  
CHOLESKY DECOMPOSITION.

SUBSECTION: CHLDEC2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"PROCEDURE" CHLDEC2(A, N, AUX); "VALUE" N; "INTEGER" N;  
"ARRAY" A, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;

"ARRAY" A[1:N, 1:N];

ENTRY: THE UPPER TRIANGLE OF THE POSITIVE DEFINITE MATRIX MUST BE GIVEN IN THE UPPER-TRIANGULAR PART OF A (THE ELEMENTS  $A[I, J]$ ,  $I \leq J$ );

EXIT: THE CHOLESKY DECOMPOSITION OF THE MATRIX IS DELIVERED IN THE UPPER TRIANGLE OF A;

N: <ARITHMETIC EXPRESSION>;

THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;

"ARRAY" AUX[2:3];

ENTRY: AUX[2]: A RELATIVE TOLERANCE USED TO CONTROL THE CALCULATION OF THE DIAGONAL ELEMENTS;

NORMAL EXIT: AUX[3] := N;

ABNORMAL EXIT: IF THE DECOMPOSITION CANNOT BE CARRIED OUT BECAUSE THE MATRIX IS (NUMERICALLY) NOT POSITIVE DEFINITE, AUX[3] := K - 1, WHERE K IS THE LAST STAGE NUMBER.

SECTION: 3,1.1.1.1.2.1

(MAY 1974)

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PROCEDURES USED: TAMMAT = CP34014.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

CHLDEC2 PERFORMS THE CHOLESKY DECOMPOSITION OF A SYMMETRIC POSITIVE DEFINITE MATRIX. THE METHOD USED IS CHOLESKY'S SQUARE ROOT METHOD WITHOUT PIVOTING (SEE REF [1] AND [2]). IF THE GIVEN SYMMETRIC MATRIX IS POSITIVE DEFINITE, THE METHOD YIELDS AN UPPER-TRIANGULAR MATRIX U SUCH THAT  $U^T U$  EQUALS THE GIVEN MATRIX. THE PROCESS IS TERMINATED AT STAGE K, IF THE K-TH DIAGONAL ELEMENT OF THE GIVEN MATRIX MINUS THE SUM OF THE SQUARED ELEMENTS OF THE K-TH COLUMN OF U IS LESS THAN A TOLERANCE TIMES THE MAXIMUM DIAGONAL ELEMENT OF THE GIVEN MATRIX. IN THIS CASE THE MATRIX, POSSIBLY MODIFIED BY ROUNDING ERRORS, IS NOT POSITIVE DEFINITE.

REFERENCES:

- [1]. T.J. DEKKER,  
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MC TRACT 22, 1968, MATH. CENTR., AMSTERDAM.
- [2]. J.H. WILKINSON,  
THE ALGEBRAIC EIGENVALUE PROBLEM,  
CLARENDON PRESS, OXFORD, 1965.

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF CHLINV2, SECTION 3,1.1.1.1,2.4.

SECTION: 3.1.1.1.1.2.1

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SUBSECTION: CHLDEC1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" CHLDEC1(A, N, AUX); "VALUE" N; "INTEGER" N;  
 "ARRAY" A, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1 : (N + 1) \* N // 2];  
 ENTRY: THE UPPER-TRIANGULAR PART OF THE POSITIVE DEFINITE SYMMETRIC MATRIX MUST BE GIVEN COLUMNWISE IN ARRAY A (THE (I,J)-TH ELEMENT OF THE MATRIX MUST BE GIVEN IN A[(J - 1) \* J // 2 + I] FOR 1 <= I <= J <= N);  
 EXIT: THE CHOLESKY DECOMPOSITION OF THE MATRIX IS DELIVERED COLUMNWISE IN A.

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[2:3];  
 ENTRY: AUX[2]: A RELATIVE TOLERANCE USED TO CONTROL THE CALCULATION OF THE DIAGONAL ELEMENTS;  
 NORMAL EXIT: AUX[3]:= N;  
 ABNORMAL EXIT: IF THE DECOMPOSITION CANNOT BE CARRIED OUT BECAUSE THE MATRIX IS (NUMERICALLY) NOT POSITIVE DEFINITE, AUX[3]:= K - 1, WHERE K IS THE LAST STAGE NUMBER.

PROCEDURES USED: VECVEC = CP34010.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

CHLDEC1 PERFORMS THE CHOLESKY DECOMPOSITION OF A SYMMETRIC POSITIVE DEFINITE MATRIX, WHOSE UPPER TRIANGLE IS STORED IN A ONE-DIMENSIONAL ARRAY, BY CHOLESKY'S SQUARE ROOT METHOD WITHOUT PIVOTING.

SEE ALSO METHOD AND PERFORMANCE OF CHLDEC2, (THIS SECTION).

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF CHLINV1, SECTION 3.1.1.1.1.2.4.



SECTION: 3.1.1.1.1.2.1

(DECEMBER 1975)

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SOURCE TEXT(S) :

```

"CODE" 34310;
"PROCEDURE" CHLDEC2(A, N, AUX); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX;
"BEGIN" "INTEGER" K, J; "REAL" R, EPSNORM;
"REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B); "CODE" 34014;

R:= 0;
"FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
"IF" A[K,K] > R "THEN" R:= A[K,K];
EPSNORM:= AUX[2] * R;
"FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" R:= A[K,K] - TAMMAT(1, K - 1, K, K, A, A);
"IF" R <= EPSNORM "THEN"
"BEGIN" AUX[3]:= K - 1; "GOTO" END "END";
A[K,K]:= R:= SQRT(R);
"FOR" J:= K + 1 "STEP" 1 "UNTIL" N "DO"
A[K,J]:= (A[K,J] - TAMMAT(1, K - 1, J, K, A, A)) / R
"END";
AUX[3]:= N;
END;
"END" CHLDEC2;
"EOP"

"CODE" 34311;
"PROCEDURE" CHLDEC1(A, N, AUX); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX;
"BEGIN" "INTEGER" J, K, KK, KJ, LOW, UP; "REAL" R, EPSNORM;
"REAL" "PROCEDURE" VECVEC(L, U, SHIFT, A, B); "CODE" 34010;

R:= 0; KK:= 0;
"FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" KK:= KK + K; "IF" A[KK] > R "THEN" R:= A[KK] "END";
EPSNORM:= AUX[2] * R; KK:= 0;
"FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" KK:= KK + K; LOW:= KK - K + 1; UP:= KK - 1;
R:= A[KK] - VECVEC(LOW, UP, 0, A, A);
"IF" R <= EPSNORM "THEN"
"BEGIN" AUX[3]:= K - 1; "GOTO" END "END";
A[KK]:= R:= SQRT(R); KJ:= KK + K;
"FOR" J:= K + 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" A[KJ]:= (A[KJ] -
VECVEC(LOW, UP, KJ - KK, A, A)) / R;
KJ:= KJ + J
"END"
"END";
AUX[3]:= N;
END;
"END" CHLDEC1;
"EOP"

```

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INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED: 731015.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS TWO PROCEDURES:

A) CHLDETERM2, FOR THE CALCULATION OF THE DETERMINANT OF A SYMMETRIC POSITIVE DEFINITE MATRIX WHOSE CHOLESKY MATRIX IS GIVEN IN A ONE-DIMENSIONAL ARRAY;

B) CHLDETERM1, FOR THE CALCULATION OF THE DETERMINANT OF A SYMMETRIC POSITIVE DEFINITE MATRIX WHOSE CHOLESKY MATRIX IS GIVEN COLUMNWISE IN A ONE-DIMENSIONAL ARRAY.

KEYWORDS:

DETERMINANT,  
POSITIVE DEFINITE SYMMETRIC MATRIX,  
CHOLESKY DECOMPOSITION.

SUBSECTION: CHLDETERM2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"REAL" "PROCEDURE" CHLDETERM2(A, N); "VALUE" N; "INTEGER" N;  
"ARRAY" A;

CHLDETERM2 DELIVERS THE DETERMINANT OF THE SYMMETRIC POSITIVE DEFINITE MATRIX OF WHICH THE CHOLESKY MATRIX IS STORED IN A;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1:N,1:N];

ENTRY: THE UPPER-TRIANGULAR PART OF THE CHOLESKY MATRIX AS PRODUCED BY CHLDEC2, SECTION 3.1.1.1.1.2.1., OR CHLDECSOL2, SECTION 3.1.1.1.1.2.3., MUST BE GIVEN IN THE UPPER TRIANGLE OF A;

EXIT: THE CONTENTS OF A ARE NOT CHANGED;

N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE MATRIX.

SECTION: 3.1.1.1.1.2.2

(MAY 1974)

PAGE 2

PROCEDURES USED: NONE.

RUNNING TIME: PROPORTIONAL TO N.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE CHLDETERM2 SHOULD BE CALLED AFTER A SUCCESSFUL CALL OF CHLDEC2 OR CHLDECSOL2, I.E. IF AUX[3] = N;  
CHLDETERM2 SHOULD NOT BE CALLED IF OVERFLOW IS TO BE EXPECTED.

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF CHLDECINV2, SECTION 3.1.1.1.1.2.4.

SUBSECTION: CHLDETERM1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
"REAL" "PROCEDURE" CHLDETERM1(A, N); "VALUE" N; "INTEGER" N;  
"ARRAY" A;

CHLDETERM1 DELIVERS THE DETERMINANT OF THE SYMMETRIC POSITIVE DEFINITE MATRIX OF WHICH THE CHOLESKY MATRIX IS STORED IN A;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1 : (N + 1) \* N // 2];  
ENTRY: THE UPPER-TRIANGULAR PART OF THE CHOLESKY MATRIX AS PRODUCED BY CHLDEC1, SECTION 3.1.1.1.1.2.1., OR CHLDECSOL1, SECTION 3.1.1.1.1.2.3., MUST BE GIVEN COLUMNWISE IN ARRAY A;  
EXIT: THE CONTENTS OF A ARE NOT CHANGED;  
N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE MATRIX.

SECTION: 3.1.1.1.1.2.2

(MAY 1974)

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PROCEDURES USED: NONE.

RUNNING TIME: PROPORTIONAL TO N.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE CHLDETERM1 SHOULD BE CALLED AFTER A SUCCESSFUL CALL OF CHLDEC1 OR CHLDECSOL1, I.E. IF AUX[3] = N; CHLDETERM1 SHOULD NOT BE CALLED IF OVERFLOW IS TO BE EXPECTED.

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF CHLDECINV1, SECTION 3.1.1.1.1.2.4.

SOURCE TEXT(S) :

```
"CODE" 34312;
  "REAL" "PROCEDURE" CHLDETERM2(A, N); "VALUE" N; "INTEGER" N;
  "ARRAY" A;
  "BEGIN" "INTEGER" K; "REAL" D;
    D:= 1;
    "FOR" K:= 1 "STEP" 1 "UNTIL" N "DO" D:= A[K,K] * D;
    CHLDETERM2:= D * D
  "END" CHLDETERM2;
  "EOP"
```

```
"CODE" 34313;
  "REAL" "PROCEDURE" CHLDETERM1(A, N); "VALUE" N; "INTEGER" N;
  "ARRAY" A;
  "BEGIN" "INTEGER" K, KK; "REAL" D;
    D:= 1; KK:= 0;
    "FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" KK:= KK + K; D:= A[KK] * D "END";
    CHLDETERM1:= D * D
  "END" CHLDETERM1;
  "EOP"
```

SECTION: 3.1.1.1.1.2.3

(MAY 1974)

PAGE 1

AUTHOR: T. J. DEKKER.

CONTRIBUTORS: S. P. N. VAN KAMPEN, J. KOK.

INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED: 731015.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS FOUR PROCEDURES;

A) CHLSOL2, FOR THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS IF THE COEFFICIENT MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE CHLDEC2, SECTION 3.1.1.1.1.2.1., OR CHLDECSOL2;

B) CHLSOL1, FOR THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS IF THE COEFFICIENT MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE CHLDEC1, SECTION 3.1.1.1.1.2.1., OR CHLDECSOL1;

C) CHLDECSOL2, FOR THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS BY CHOLESKY'S SQUARE ROOT METHOD;  
THE COEFFICIENT MATRIX HAS TO BE SYMMETRIC POSITIVE DEFINITE AND MUST BE GIVEN IN THE UPPER TRIANGLE OF A TWO-DIMENSIONAL ARRAY;

D) CHLDECSOL1, FOR THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS BY CHOLESKY'S SQUARE ROOT METHOD;  
THE COEFFICIENT MATRIX HAS TO BE SYMMETRIC POSITIVE DEFINITE AND MUST BE GIVEN COLUMNWISE IN A ONE-DIMENSIONAL ARRAY.

KEYWORDS:

LINEAR EQUATIONS,  
POSITIVE DEFINITE SYMMETRIC MATRIX,  
CHOLESKY DECOMPOSITION.

SUBSECTION: CHLSOL2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" CHLSOL2(A, N, B); "VALUE" N; "INTEGER" N; "ARRAY" A, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE UPPER-TRIANGULAR PART OF THE CHOLESKY MATRIX  
 AS PRODUCED BY CHLDEC2, SECTION 3.1.1.1.1.2.1., OR  
 CHLDECSOL2 (THIS SECTION), MUST BE GIVEN IN THE  
 UPPER TRIANGLE OF A;  
 EXIT: THE CONTENTS OF A ARE NOT CHANGED;  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;  
 B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR  
 EQUATIONS;  
 EXIT: THE SOLUTION OF THE SYSTEM.

PROCEDURES USED:

MATVEC = CP34011,  
 TAMVEC = CP34012.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N SQUARED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE CHLSOL2 CALCULATES THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS, PROVIDED THAT THE COEFFICIENT MATRIX HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF CHLDEC2 OR CHLDECSOL2; THE SOLUTION IS OBTAINED BY CARRYING OUT THE FORWARD AND BACK SUBSTITUTION WITH THE CHOLESKY MATRIX AND THE RIGHT HAND SIDE. THE RIGHT HAND SIDE IS OVERWRITTEN BY THE SOLUTION BUT THE ELEMENTS OF THE CHOLESKY MATRIX ARE NOT CHANGED, THUS SEVERAL SYSTEMS OF LINEAR EQUATIONS WITH THE SAME COEFFICIENT MATRIX BUT DIFFERENT RIGHT HAND SIDES CAN BE SOLVED BY SUCCESSIVE CALLS OF CHLSOL2. SEE ALSO REF [1].

REFERENCES:

[1], T.J. DEKKER,  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 1,  
 MC TRACT 22, 1968, MATH. CENTR., AMSTERDAM.

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF CHLINV2, SECTION 3.1.1.1.1.2.4.

SUBSECTION: CHLSOL1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
"PROCEDURE" CHLSOL1(A, N, B); "VALUE" N; "INTEGER" N; "ARRAY" A, B;

THE MEANING OF THE FORMAL PARAMETERS IS:  
A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1 : (N + 1) \* N // 2];  
ENTRY: THE UPPER-TRIANGULAR PART OF THE CHOLESKY MATRIX  
AS PRODUCED BY CHLDEC1, SECTION 3.1.1.1.1.2.1., OR  
CHLDECSOL1 (THIS SECTION), MUST BE GIVEN COLUMNWISE  
IN ARRAY A;  
EXIT: THE CONTENTS OF A ARE NOT CHANGED;  
N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE MATRIX;  
B: <ARRAY IDENTIFIER>;  
"ARRAY" B[1:N];  
ENTRY: THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR  
EQUATIONS;  
EXIT: THE SOLUTION OF THE SYSTEM.

PROCEDURES USED:

VECVEC = CP34010,  
SEQVEC = CP34016.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N SQUARED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE CHLSOL1 CALCULATES THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS, PROVIDED THAT THE COEFFICIENT MATRIX HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF CHLDEC1 OR CHLDECSOL1; SEVERAL SYSTEMS WITH THE SAME COEFFICIENT MATRIX BUT DIFFERENT RIGHT HAND SIDES CAN BE SOLVED BY SUCCESSIVE CALLS OF CHLSOL1. SEE ALSO METHOD AND PERFORMANCE OF CHLSOL2 (THIS SECTION).

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF CHLINV1, SECTION 3.1.1.1.1.2.4.

SECTION: 3.1.1.1.1.2.3

(DECEMBER 1975)

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SUBSECTION: CHLDECSOL2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" CHLDECSOL2(A, N, AUX, B); "VALUE" N; "INTEGER" N;  
 "ARRAY" A, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE UPPER TRIANGLE OF THE POSITIVE DEFINITE MATRIX  
 MUST BE GIVEN IN THE UPPER-TRIANGULAR PART OF A (THE  
 ELEMENTS A[I,J], I <= J);  
 EXIT: THE CHOLESKY DECOMPOSITION OF THE MATRIX IS  
 DELIVERED IN THE UPPER TRIANGLE OF A;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[2:3];  
 ENTRY: AUX[2]: A RELATIVE TOLERANCE USED TO CONTROL THE  
 CALCULATION OF THE DIAGONAL ELEMENTS; (SEE METHOD  
 AND PERFORMANCE OF CHLDEC2, SECTION 3.1.1.1.1.2.1);  
 NORMAL EXIT: AUX[3]:= N;  
 ABNORMAL EXIT: IF THE DECOMPOSITION CANNOT BE CARRIED OUT  
 BECAUSE THE MATRIX IS (NUMERICALLY) NOT POSITIVE  
 DEFINITE, AUX[3]:= K - 1, WHERE K IS THE LAST STAGE  
 NUMBER.

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR  
 EQUATIONS;  
 EXIT: THE SOLUTION OF THE SYSTEM.

PROCEDURES USED:

CHLDEC2 = CP34310,  
 CHLSOL2 = CP34390.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE CHLDECSOL2 SOLVES A SYSTEM OF LINEAR EQUATIONS WITH  
 A SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX BY CALLING  
 CHLDEC2, SECTION 3.1.1.1.1.2.1., AND, IF THIS CALL WAS  
 SUCCESSFUL, CHLSOL2 (THIS SECTION).  
 SEE ALSO CHLDEC2, SECTION 3.1.1.1.1.2.1.

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF CHLDECINV2, SECTION 3.1.1.1.1.2.4.



SECTION: 3.1.1.1.1.2.3

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SUBSECTION: CHLDECSOL1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" CHLDECSOL1(A, N, AUX, B); "VALUE" N; "INTEGER" N;  
 "ARRAY" A, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1 : (N + 1) \* N // 2];  
 ENTRY: THE UPPER-TRIANGULAR PART OF THE POSITIVE DEFINITE SYMMETRIC MATRIX MUST BE GIVEN COLUMNWISE IN ARRAY A (THE (I, J)-TH ELEMENT OF THE MATRIX MUST BE GIVEN IN A[(J - 1) \* J // 2 + I] FOR 1 <= I <= J <= N);  
 EXIT: THE CHOLESKY DECOMPOSITION OF THE MATRIX IS DELIVERED COLUMNWISE IN A.

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[2:3];  
 ENTRY: AUX[2]: A RELATIVE TOLERANCE USED TO CONTROL THE CALCULATION OF THE DIAGONAL ELEMENTS;  
 NORMAL EXIT: AUX[3]:= N;  
 ABNORMAL EXIT: IF THE DECOMPOSITION CANNOT BE CARRIED OUT BECAUSE THE MATRIX IS (NUMERICALLY) NOT POSITIVE DEFINITE, AUX[3]:= K - 1, WHERE K IS THE LAST STAGE NUMBER.

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR EQUATIONS;  
 EXIT: THE SOLUTION OF THE SYSTEM.

PROCEDURES USED:

CHLDEC1 = CP34311,  
 CHLSOL1 = CP34391.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE CHLDECSOL1 SOLVES A SYSTEM OF LINEAR EQUATIONS WITH A SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX BY CALLING CHLDEC1, SECTION 3.1.1.1.1.2.1., AND, IF THIS CALL WAS SUCCESSFUL, CHLSOL1 (THIS SECTION).  
 THE UPPER TRIANGLE OF THE COEFFICIENT MATRIX MUST BE STORED COLUMNWISE IN A ONE-DIMENSIONAL ARRAY.  
 SEE ALSO CHLDEC1, SECTION 3.1.1.1.1.2.1.

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF CHLDECINV1, SECTION 3.1.1.1.1.2.4.

## SOURCE TEXT(S) :

```

"CODE" 34390;
  "PROCEDURE" CHLSOL2(A, N, B); "VALUE" N; "INTEGER" N; "ARRAY" A, B;
  "BEGIN" "INTEGER" I;
    "REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
    "REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;

    "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
      B[I]:= (B[I] - TAMVEC(1, I - 1, I, A, B)) / A[I,I];
    "FOR" I:= N "STEP" - 1 "UNTIL" 1 "DO"
      B[I]:= (B[I] - MATVEC(I + 1, N, I, A, B)) / A[I,I]
  "END" CHLSOL2;
  "EOP"
"CODE" 34391;
  "PROCEDURE" CHLSOL1(A, N, B); "VALUE" N; "INTEGER" N; "ARRAY" A, B;
  "BEGIN" "INTEGER" I, II;
    "REAL" "PROCEDURE" VECVEC(L, U, SHIFT, A, B); "CODE" 34010;
    "REAL" "PROCEDURE" SEQVEC(L, U, I1, SHIFT, A, B); "CODE" 34016;

    II:= 0;
    "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" II:= II + I;
        B[II]:= (B[II] - VECVEC(1, I - 1, II - I, B, A)) / A[II]
      "END";
    "FOR" I:= N "STEP" - 1 "UNTIL" 1 "DO"
      "BEGIN" B[I]:= (B[I] -
        SEQVEC(I + 1, N, II + I, 0, A, B)) / A[II];
        II:= II - I
      "END"
  "END" CHLSOL1;
  "EOP"
"CODE" 34392;
  "PROCEDURE" CHLDECSOL2(A, N, AUX, B); "VALUE" N; "INTEGER" N;
  "ARRAY" A, AUX, B;
  "BEGIN"
    "PROCEDURE" CHLDEC2(A, N, AUX); "CODE" 34310;
    "PROCEDURE" CHLSOL2(A, N, B); "CODE" 34390;

    CHLDEC2(A, N, AUX);
    "IF" AUX[3] = N "THEN" CHLSOL2(A, N, B)
  "END" CHLDECSOL2;
  "EOP"
"CODE" 34393;
  "PROCEDURE" CHLDECSOL1(A, N, AUX, B); "VALUE" N; "INTEGER" N;
  "ARRAY" A, AUX, B;
  "BEGIN"
    "PROCEDURE" CHLDEC1(A, N, AUX); "CODE" 34311;
    "PROCEDURE" CHLSOL1(A, N, B); "CODE" 34391;

    CHLDEC1(A, N, AUX);
    "IF" AUX[3] = N "THEN" CHLSOL1(A, N, B)
  "END" CHLDECSOL1;
  "EOP"

```

SECTION: 3.1.1.1.1.2.4

(MAY 1974)

PAGE 1

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INSTITUTE: MATHEMATICAL CENTRE,

RECEIVED: 731015,

BRIEF DESCRIPTION:

THIS SECTION CONTAINS FOUR PROCEDURES:

A) CHLINV2, FOR THE INVERSION OF A SYMMETRIC POSITIVE DEFINITE MATRIX, IF THE MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE CHLDEC2, SECTION 3.1.1.1.1.2.1., OR CHLDECSOL2, SECTION 3.1.1.1.1.2.3.;

B) CHLINV1, FOR THE INVERSION OF A SYMMETRIC POSITIVE DEFINITE MATRIX, IF THE MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE CHLDEC1, SECTION 3.1.1.1.1.2.1., OR CHLDECSOL1, SECTION 3.1.1.1.1.2.3.;

C) CHLDECINV2, FOR THE INVERSION OF A MATRIX BY CHOLESKY'S SQUARE ROOT METHOD;

THE COEFFICIENT MATRIX HAS TO BE SYMMETRIC POSITIVE DEFINITE AND MUST BE GIVEN IN THE UPPER TRIANGLE OF A TWO-DIMENSIONAL ARRAY;

D) CHLDECINV1, FOR THE INVERSION OF A MATRIX BY CHOLESKY'S SQUARE ROOT METHOD;

THE COEFFICIENT MATRIX HAS TO BE SYMMETRIC POSITIVE DEFINITE AND MUST BE GIVEN COLUMNWISE IN A ONE-DIMENSIONAL ARRAY.

KEYWORDS:

MATRIX INVERSION,  
 POSITIVE DEFINITE SYMMETRIC MATRIX,  
 CHOLESKY DECOMPOSITION.

SECTION: 3.1.1.1.1.2.4

(MAY 1974)

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SUBSECTION: CHLINV2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" CHLINV2(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE UPPER-TRIANGULAR PART OF THE CHOLESKY MATRIX  
 AS PRODUCED BY CHLDEC2, SECTION 3.1.1.1.1.2.1., OR  
 CHLDECSOL2, SECTION 3.1.1.1.1.2.3., MUST BE GIVEN  
 IN THE UPPER TRIANGLE OF A;  
 EXIT: THE UPPER-TRIANGULAR PART OF THE INVERSE MATRIX IS  
 DELIVERED IN THE UPPER TRIANGLE OF A;  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX.

PROCEDURES USED:

MATVEC = CP34011,  
 TAMVEC = CP34012,  
 DUPVECROW = CP31031.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: N.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE CHLINV2 CALCULATES THE INVERSE OF A MATRIX, PROVIDED  
 THAT THE MATRIX HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF CHLDEC2  
 OR CHLDECSOL2;  
 THE INVERSE, X, OF U<sup>T</sup>U, WHERE U IS THE CHOLESKY MATRIX,  
 IS OBTAINED FROM THE CONDITIONS THAT X BE SYMMETRIC AND UX BE  
 A LOWER-TRIANGULAR MATRIX WHOSE MAIN DIAGONAL ELEMENTS ARE THE  
 RECIPROCAL OF THE DIAGONAL ELEMENTS OF U, HEREWITH THE UPPER-  
 TRIANGULAR ELEMENTS OF X ARE CALCULATED BY BACK SUBSTITUTION,  
 THE UPPER TRIANGLE OF THE INVERSE MATRIX IS DELIVERED IN THE UPPER  
 TRIANGLE OF THE GIVEN ARRAY, SEE ALSO REF [1].

REFERENCES:

- [1]. T.J. DEKKER,  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 1,  
 MC TRACT 22, 1968, MATH. CENTR., AMSTERDAM.

## EXAMPLE OF USE:

THE SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX (THE PASCAL MATRIX OF ORDER 4) OF THE SYSTEM OF EQUATIONS

$$X_1 + X_2 + X_3 + X_4 = 2$$

$$X_1 + 2 * X_2 + 3 * X_3 + 4 * X_4 = 4$$

$$X_1 + 3 * X_2 + 6 * X_3 + 10 * X_4 = 8$$

$$X_1 + 4 * X_2 + 10 * X_3 + 20 * X_4 = 16$$

IS STORED IN THE TWO-DIMENSIONAL ARRAY PASCAL2.

THE INVERSE OF THE COEFFICIENT MATRIX AND THE SOLUTION OF THE LINEAR SYSTEM ARE CALCULATED BY THE FOLLOWING PROGRAM:

```
"BEGIN" "COMMENT" TEST CHLDEC2, CHLSOL2 AND CHLINV2;
  "INTEGER" I, J;
  "ARRAY" PASCAL2[1:4,1:4], B[1:4], AUX[2:3];
  "PROCEDURE" CHLDEC2(A, N, AUX); "CODE" 34310;
  "PROCEDURE" CHLSOL2(A, N, B); "CODE" 34390;
  "PROCEDURE" CHLINV2(A, N); "CODE" 34400;
  "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" PASCAL2[I,J]:= 1;
    "FOR" I:= 2 "STEP" 1 "UNTIL" J "DO"
      PASCAL2[I,J]:= "IF" I = J "THEN" PASCAL2[I-1,J] * 2 "ELSE"
        PASCAL2[I,J-1] + PASCAL2[I-1,J];
    B[J]:= 2 ** J
  "END";
  AUX[2]:= "-11;
  CHLDEC2(PASCAL2, 4, AUX);
  "IF" AUX[3] = 4 "THEN"
  "BEGIN" CHLSOL2(PASCAL2, 4, B); CHLINV2(PASCAL2, 4) "END"
  "ELSE" OUTPUT(61, "("("MATRIX NOT POSITIVE DEFINITE")", /")");
  OUTPUT(61, "("4B")");
  OUTPUT(61, "("("SOLUTION WITH CHLDEC2 AND CHLSOL2:", /")");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  OUTPUT(61, "("4B+D,5D")", B[I]);
  OUTPUT(61, "("//, 4B")");
  OUTPUT(61, "("("INVERSE MATRIX WITH CHLINV2:", /, 4B")");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    "IF" J < I "THEN" OUTPUT(61, "("12B")") "ELSE"
    OUTPUT(61, "("+ZD,5D3B")", PASCAL2[I,J]);
    OUTPUT(61, "("/, 4B")");
  "END"
"END"
```

## THIS PROGRAM DELIVERS:

SOLUTION WITH CHLDEC2 AND CHLSOL2:

+0.00000	+4.00000	-4.00000	+2.00000
----------	----------	----------	----------

INVERSE MATRIX WITH CHLINV2:

+4.00000	-6.00000	+4.00000	-1.00000
	+14.00000	-11.00000	+3.00000
		+10.00000	-3.00000
			+1.00000

SECTION: 3.1.1.1.1.2.4

(MAY 1974)

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SUBSECTION: CHLINV1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" CHLINV1(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:(N + 1) \* N // 2];  
 ENTRY: THE UPPER-TRIANGULAR PART OF THE CHOLESKY MATRIX  
 AS PRODUCED BY CHLDEC1, SECTION 3.1.1.1.1.2.1., OR  
 CHLDECSOL1, SECTION 3.1.1.1.1.2.3., MUST BE GIVEN  
 COLUMNWISE IN ARRAY A;  
 EXIT: THE UPPER-TRIANGULAR PART OF THE INVERSE MATRIX IS  
 DELIVERED COLUMNWISE IN ARRAY A;  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX.

PROCEDURES USED:

SEQVEC = CP34016,  
 SYMMATVEC = CP34018,

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: N.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE CHLINV1 CALCULATES THE INVERSE OF A MATRIX, PROVIDED  
 THAT THE MATRIX HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF CHLDEC1  
 OR CHLDECSOL1;  
 THE UPPER TRIANGLE OF THE INVERSE MATRIX IS DELIVERED COLUMNWISE  
 IN THE ONE-DIMENSIONAL ARRAY.  
 SEE ALSO METHOD AND PERFORMANCE OF CHLINV2 (THIS SECTION).

EXAMPLE OF USE:

THE SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX (THE PASCAL  
 MATRIX OF ORDER 4) OF THE SYSTEM OF EQUATIONS

$$x_1 + x_2 + x_3 + x_4 = 2$$

$$x_1 + 2 * x_2 + 3 * x_3 + 4 * x_4 = 4$$

$$x_1 + 3 * x_2 + 6 * x_3 + 10 * x_4 = 8$$

$$x_1 + 4 * x_2 + 10 * x_3 + 20 * x_4 = 16$$

IS STORED IN THE ONE-DIMENSIONAL ARRAY PASCAL1.  
 THE INVERSE OF THE COEFFICIENT MATRIX AND THE SOLUTION OF THE  
 LINEAR SYSTEM ARE CALCULATED BY THE FOLLOWING PROGRAM:

```

"BEGIN" "COMMENT" TEST CHLDEC1, CHLSOL1 AND CHLINV1;
  "INTEGER" I, J, JJ;
  "ARRAY" PASCAL1[1:(4 + 1) * 4 // 2], B[1:4], AUX[2:3];

  "PROCEDURE" CHLDEC1(A, N, AUX); "CODE" 34311;
  "PROCEDURE" CHLSOL1(A, N, B); "CODE" 34391;
  "PROCEDURE" CHLINV1(A, N); "CODE" 34401;

  JJ:= 1;
  "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" PASCAL1[JJ]:= 1;
    "FOR" I:= 2 "STEP" 1 "UNTIL" J "DO"
    PASCAL1[JJ + I - 1]:= "IF" I = J "THEN"
    PASCAL1[JJ + I - 2] * 2 "ELSE"
    PASCAL1[JJ + I - 2] + PASCAL1[JJ + I - J];
    B[J]:= 2 ** J;
    JJ:= JJ + J
  "END";

  AUX[2]:= "-11";
  CHLDEC1(PASCAL1, 4, AUX);
  "IF" AUX[3] = 4 "THEN"
  "BEGIN" CHLSOL1(PASCAL1, 4, B); CHLINV1(PASCAL1, 4) "END"
  "ELSE" OUTPUT(61, "("("MATRIX NOT POSITIVE DEFINITE"), "/"");

  OUTPUT(61, "("4B");
  OUTPUT(61, "("("SOLUTION WITH CHLDEC1 AND CHLSOL1:"), "/"");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  OUTPUT(61, "("4B+D,5D"), B[I]);
  OUTPUT(61, "("2/, 4B");
  OUTPUT(61, "("("INVERSE MATRIX WITH CHLINV1:"), /, 4B");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    "IF" J < I "THEN" OUTPUT(61, "("12B")" "ELSE"
    OUTPUT(61, "("+ZD,5D3B"), PASCAL1[(J - 1) * J // 2 + I]);
    OUTPUT(61, "("/, 4B");
  "END"
"END"

```

THIS PROGRAM DELIVERS:

SOLUTION WITH CHLDEC1 AND CHLSOL1:

+0,00000	+4,00000	=4,00000	+2,00000
----------	----------	----------	----------

INVERSE MATRIX WITH CHLINV1:

+4,00000	-6,00000	+4,00000	=1,00000
	+14,00000	=11,00000	+3,00000
		+10,00000	=3,00000
			+1,00000

SECTION: 3.1.1.1.1.2.4

(MAY 1974)

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SUBSECTION: CHLDECINV2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
"PROCEDURE" CHLDECINV2(A, N, AUX); "VALUE" N; "INTEGER" N;  
"ARRAY" A, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1:N,1:N];  
ENTRY: THE UPPER TRIANGLE OF THE POSITIVE DEFINITE MATRIX  
MUST BE GIVEN IN THE UPPER TRIANGLE OF A (THE  
ELEMENTS A[I,J], I ≤ J);  
EXIT: THE UPPER-TRIANGULAR PART OF THE INVERSE MATRIX IS  
DELIVERED IN THE UPPER TRIANGLE OF A.  
N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE MATRIX;  
AUX: <ARRAY IDENTIFIER>;  
"ARRAY" AUX[2:3];  
ENTRY: AUX[2]; A RELATIVE TOLERANCE USED TO CONTROL THE  
CALCULATION OF THE DIAGONAL ELEMENTS;  
NORMAL EXIT: AUX[3] = N;  
ABNORMAL EXIT: IF THE DECOMPOSITION CANNOT BE CARRIED OUT  
BECAUSE THE MATRIX IS (NUMERICALLY) NOT POSITIVE  
DEFINITE, AUX[3] = K - 1, WHERE K IS THE LAST STAGE  
NUMBER.

PROCEDURES USED:

CHLDEC2 = CP34310,  
CHLINV2 = CP34400.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE CHLDECINV2 CALCULATES THE INVERSE OF A SYMMETRIC  
POSITIVE DEFINITE MATRIX BY CALLING CHLDEC2 AND, IF THIS CALL WAS  
SUCCESSFUL, CHLINV2.  
THE UPPER TRIANGLE OF THE INVERSE MATRIX IS DELIVERED IN THE UPPER  
TRIANGLE OF THE GIVEN ARRAY.  
SEE ALSO METHOD AND PERFORMANCE OF CHLINV2 (THIS SECTION) AND  
CHLDEC2, SECTION 3.1.1.1.1.2.1.



## EXAMPLE OF USE:

THE SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX (THE PASCAL MATRIX OF ORDER 4) OF THE SYSTEM OF EQUATIONS

$$\begin{array}{r} X_1 + \quad X_2 + \quad X_3 + \quad X_4 = 2 \\ X_1 + 2 * X_2 + 3 * X_3 + 4 * X_4 = 4 \\ X_1 + 3 * X_2 + 6 * X_3 + 10 * X_4 = 8 \\ X_1 + 4 * X_2 + 10 * X_3 + 20 * X_4 = 16 \end{array}$$

IS STORED IN THE TWO-DIMENSIONAL ARRAY PASCAL2.  
THE DETERMINANT AND THE INVERSE OF THE COEFFICIENT MATRIX AND THE SOLUTION OF THE LINEAR SYSTEM ARE CALCULATED BY THE FOLLOWING PROGRAM:

```

"BEGIN" "COMMENT" TEST CHLDECSOL2, CHLDETERM2 AND CHLDECINV2;
  "INTEGER" I, J;
  "ARRAY" PASCAL2[1:4,1:4], B[1:4], AUX[2:3];
  "REAL" DETERMINANT;
  "PROCEDURE" CHLDECSOL2(A, N, AUX, B); "CODE" 34392;
  "REAL" "PROCEDURE" CHLDETERM2(A, N); "CODE" 34312;
  "PROCEDURE" CHLDECINV2(A, N, AUX); "CODE" 34402;
  "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" PASCAL2[1,J]:= 1;
    "FOR" I:= 2 "STEP" 1 "UNTIL" J "DO"
      PASCAL2[I,J]:= "IF" I = J "THEN" PASCAL2[I-1,J] * 2 "ELSE"
        PASCAL2[I,J-1] + PASCAL2[I-1,J];
    B[J]:= 2 ** J
  "END";
  AUX[2]:= "-11;
  CHLDECSOL2(PASCAL2, 4, AUX, B);
  "IF" AUX[3] = 4 "THEN" DETERMINANT:= CHLDETERM2(PASCAL2, 4)
  "ELSE" OUTPUT(61, "("("MATRIX NOT POSITIVE DEFINITE")", /(")");
  OUTPUT(61, "("("4B")");
  OUTPUT(61, "("("SOLUTION WITH CHLDECSOL2:")", /(")");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  OUTPUT(61, "("("4B+D.5D")", B[I]);
  OUTPUT(61, "("(/, 4B, "("("DETERMINANT WITH CHLDETERM2: ")",
    +D.5D, 2/, 4B")", DETERMINANT);
  "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" PASCAL2[1,J]:= 1;
    "FOR" I:= 2 "STEP" 1 "UNTIL" J "DO"
      PASCAL2[I,J]:= "IF" I = J "THEN" PASCAL2[I-1,J] * 2 "ELSE"
        PASCAL2[I,J-1] + PASCAL2[I-1,J]
  "END";
  CHLDECINV2(PASCAL2, 4, AUX);
  OUTPUT(61, "("("INVERSE MATRIX WITH CHLDECINV2:")", /, 4B")");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    "IF" J < I "THEN" OUTPUT(61, "("("12B")") "ELSE"
      OUTPUT(61, "("("+ZD.5D3B")", PASCAL2[I,J]);
      OUTPUT(61, "("(/, 4B")")
  "END"
"END"

```

SECTION: 3.1.1.1.1.2.4

(DECEMBER 1975)

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THIS PROGRAM DELIVERS:

SOLUTION WITH CHLDECSOL2:

+0.00000      +4.00000      -4.00000      +2.00000

DETERMINANT WITH CHLDETERM2: +1.00000

INVERSE MATRIX WITH CHLDECINV2:

+4.00000	-6.00000	+4.00000	-1.00000
	+14.00000	-11.00000	+3.00000
		+10.00000	-3.00000
			+1.00000

SUBSECTION: CHLDECINV1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"PROCEDURE" CHLDECINV1(A, N, AUX); "VALUE" N; "INTEGER" N;

"ARRAY" A, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" A[1:(N + 1) \* N // 2];

ENTRY: THE UPPER-TRIANGULAR PART OF THE SYMMETRIC POSITIVE DEFINITE MATRIX MUST BE GIVEN COLUMNWISE IN ARRAY A (THE (I, J)-TH ELEMENT OF THE MATRIX MUST BE GIVEN IN A[(J - 1) \* J // 2 + I] FOR 1 &lt;= I &lt;= J &lt;= N);

EXIT: THE UPPER-TRIANGULAR PART OF THE INVERSE MATRIX IS DELIVERED COLUMNWISE IN ARRAY A;

N: &lt;ARITHMETIC EXPRESSION&gt;;

THE ORDER OF THE MATRIX;

AUX: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" AUX[2:3];

ENTRY: AUX[2]: A RELATIVE TOLERANCE USED TO CONTROL THE CALCULATION OF THE DIAGONAL ELEMENTS; (SEE METHOD AND PERFORMANCE OF CHLDEC2, SECTION 3.1.1.1.1.2.1);

NORMAL EXIT: AUX[3]:= N;

ABNORMAL EXIT: IF THE DECOMPOSITION CANNOT BE CARRIED OUT BECAUSE THE MATRIX IS (NUMERICALLY) NOT POSITIVE DEFINITE, AUX[3]:= K - 1, WHERE K IS THE LAST STAGE NUMBER.

SECTION: 3.1.1.1.1.2.4

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## PROCEDURES USED:

CHLDEC1 = CP34311,  
 CHLINV1 = CP34401.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

THE PROCEDURE CHLDECINV1 CALCULATES THE INVERSE OF A SYMMETRIC POSITIVE DEFINITE MATRIX BY CALLING CHLDEC1 AND, IF THIS CALL WAS SUCCESSFUL, CHLINV1. THE UPPER TRIANGLE OF THE INVERSE MATRIX IS DELIVERED COLUMNWISE IN THE GIVEN ONE-DIMENSIONAL ARRAY. SEE ALSO METHOD AND PERFORMANCE OF CHLINV2, (THIS SECTION) AND CHLDEC1, SECTION 3.1.1.1.1.2.1.

## EXAMPLE OF USE:

THE SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX (THE PASCAL MATRIX OF ORDER 4) OF THE SYSTEM OF EQUATIONS

$$\begin{array}{r}
 X1 + \quad X2 + \quad X3 + \quad X4 = 2 \\
 X1 + 2 * X2 + 3 * X3 + 4 * X4 = 4 \\
 X1 + 3 * X2 + 6 * X3 + 10 * X4 = 8 \\
 X1 + 4 * X2 + 10 * X3 + 20 * X4 = 16
 \end{array}$$

IS STORED IN THE ONE-DIMENSIONAL ARRAY PASCAL1. THE DETERMINANT AND THE INVERSE OF THE COEFFICIENT MATRIX AND THE SOLUTION OF THE LINEAR SYSTEM ARE CALCULATED BY THE FOLLOWING PROGRAM:

```

"BEGIN" "COMMENT" TEST CHLDECSOL1, CHLDETERM1 AND CHLDECINV1;
  "INTEGER" I, J, JJ;
  "ARRAY" PASCAL1[1:(4 + 1) * 4 // 2], B[1:4], AUX[2:3];
  "REAL" DETERMINANT;

  "PROCEDURE" CHLDECSOL1(A, N, AUX, B); "CODE" 34393;
  "REAL" "PROCEDURE" CHLDETERM1(A, N); "CODE" 34313;
  "PROCEDURE" CHLDECINV1(A, N, AUX); "CODE" 34403;

  JJ:= 1;
  "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" PASCAL1[JJ]:= 1;
    "FOR" I:= 2 "STEP" 1 "UNTIL" J "DO"
      PASCAL1[JJ + I - 1]:= "IF" I = J "THEN"
      PASCAL1[JJ + I - 2] * 2 "ELSE"
      PASCAL1[JJ + I - 2] + PASCAL1[JJ + I - J];
      B[J]:= 2 ** J;
      JJ:= JJ + J
  "END";

  AUX[2]:= "-11;
  CHLDECSOL1(PASCAL1, 4, AUX, B);
  "IF" AUX[3] = 4 "THEN" DETERMINANT:= CHLDETERM1(PASCAL1, 4)
  "ELSE" OUTPUT(61, "(" ("MATRIX NOT POSITIVE DEFINITE") ", /");

  OUTPUT(61, "(" ("4B") ");
  OUTPUT(61, "(" ("SOLUTION WITH CHLDECSOL1:"), /");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  OUTPUT(61, "(" ("4B+D.5D") ", B[I]);
  OUTPUT(61, "(" (//, 4B, ("DETERMINANT WITH CHLDETERM1: "),
    +D.5D, 2/, 4B"), DETERMINANT);

  JJ:= 1;
  "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" PASCAL1[JJ]:= 1;
    "FOR" I:= 2 "STEP" 1 "UNTIL" J "DO"
      PASCAL1[JJ + I - 1]:= "IF" I = J "THEN"
      PASCAL1[JJ + I - 2] * 2 "ELSE"
      PASCAL1[JJ + I - 2] + PASCAL1[JJ + I - J];
      JJ:= JJ + J
  "END";

  CHLDECINV1(PASCAL1, 4, AUX);

  OUTPUT(61, "(" ("INVERSE MATRIX WITH CHLDECINV1:"), /, 4B");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    "IF" J < I "THEN" OUTPUT(61, "(" ("12B") ") "ELSE"
    OUTPUT(61, "(" (+ZD.5D3B"), PASCAL1[(J - 1) * J // 2 + I]);
    OUTPUT(61, "(" (//, 4B") ")
  "END"
"END"

```

THIS PROGRAM DELIVERS:

SOLUTION WITH CHLDECSOL1:

+0.00000      +4.00000      -4.00000      +2.00000

DETERMINANT WITH CHLDETERM1: +1.00000

INVERSE MATRIX WITH CHLDECINV1:

+4.00000	-6.00000	+4.00000	-1.00000
	+14.00000	-11.00000	+3.00000
		+10.00000	-3.00000
			+1.00000

SOURCE TEXT(S) :

```
"CODE" 34400;
"PROCEDURE" CHLINV2(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;
"BEGIN" "REAL" R; "INTEGER" I, J, I1;
"ARRAY" U[1:N];
"PROCEDURE" DUPVECROW(L, U, I, A, B); "CODE" 31031;
"REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
"REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;

"FOR" I:= N "STEP" = 1 "UNTIL" 1 "DO"
"BEGIN" R:= 1 / A[I,I]; I1:= I + 1;
      DUPVECROW(I1, N, I, U, A);
      "FOR" J:= N "STEP" = 1 "UNTIL" I1 "DO" A[I,J]:=
      = (TAMVEC(I1, J, J, A, U) + MATVEC(J + 1, N, J, A, U)) * R;
      A[I,I]:= (R - MATVEC(I1, N, I, A, U)) * R
"END"
"END" CHLINV2;
"EOP"

"CODE" 34401;
"PROCEDURE" CHLINV1(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;
"BEGIN" "INTEGER" I, II, I1, J, IJ; "REAL" R;
"ARRAY" U[1:N];
"REAL" "PROCEDURE" SEQVEC(L, U, I1, SHIFT, A, B); "CODE" 34016;
"REAL" "PROCEDURE" SYMMATVEC(L, U, I, A, B); "CODE" 34018;

II:= (N + 1) * N // 2;
"FOR" I:= N "STEP" = 1 "UNTIL" 1 "DO"
"BEGIN" R:= 1 / A[II]; I1:= I + 1; IJ:= II + I;
      "FOR" J:= I1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" U[IJ]:= A[IJ]; IJ:= IJ + J "END";
      "FOR" J:= N "STEP" = 1 "UNTIL" I1 "DO"
      "BEGIN" IJ:= IJ - J; A[IJ]:= -SYMMATVEC(I1, N, J, A, U) * R
      "END";
      A[II]:= (R - SEQVEC(I1, N, II + I, 0, A, U)) * R;
      II:= II - I
"END"
"END" CHLINV1;
"EOP"
```

```
"CODE" 34402;
  "PROCEDURE" CHLDECINV2(A, N, AUX); "VALUE" N; "INTEGER" N;
  "ARRAY" A, AUX;
  "BEGIN"
    "PROCEDURE" CHLDEC2(A, N, AUX); "CODE" 34310;
    "PROCEDURE" CHLINV2(A, N); "CODE" 34400;

    CHLDEC2(A, N, AUX);
    "IF" AUX[3] = N "THEN" CHLINV2(A, N)
  "END" CHLDECINV2;
  "EQP"
```

```
"CODE" 34403;
  "PROCEDURE" CHLDECINV1(A, N, AUX); "VALUE" N; "INTEGER" N;
  "ARRAY" A, AUX;
  "BEGIN"
    "PROCEDURE" CHLDEC1(A, N, AUX); "CODE" 34311;
    "PROCEDURE" CHLINV1(A, N); "CODE" 34401;

    CHLDEC1(A, N, AUX);
    "IF" AUX[3] = N "THEN" CHLINV1(A, N)
  "END" CHLDECINV1;
  "EQP"
```

SECTION : 3.1.1.1.1.3.1

(JANUARY 1976)

PAGE 1

AUTHOR: J. KOK.

INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED: 751124.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS TWO PROCEDURES FOR THE SYMMETRIC DECOMPOSITION (THE  $U^T D U$  - DECOMPOSITION) OF A SYMMETRIC (POSSIBLY DEFINITE) MATRIX :

- A) SYMDEC2 CALCULATES THE SYMMETRIC DECOMPOSITION OF A MATRIX WHOSE UPPER TRIANGLE IS GIVEN IN A TWO-DIMENSIONAL ARRAY;
- B) SYMDEC1 CALCULATES THE SYMMETRIC DECOMPOSITION OF A MATRIX WHOSE UPPER TRIANGLE IS GIVEN COLUMNWISE IN A ONE-DIMENSIONAL ARRAY.

KEYWORDS:

LINEAR EQUATIONS,  
DEFINITE SYMMETRIC MATRIX,  
SYMMETRIC DECOMPOSITION.

SECTION : 3.1.1.1.1.3.1

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SUBSECTION: SYMDEC2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" SYMDEC2(A, N, AUX); "VALUE" N; "INTEGER" N;  
 "ARRAY" A, AUX;  
 "CODE" 34700;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : N, 1 : N];  
 ENTRY: THE UPPER TRIANGLE OF THE DEFINITE SYMMETRIC MATRIX  
 MUST BE GIVEN IN THE UPPER-TRIANGULAR PART OF A (THE  
 ELEMENTS A[I,J], I ≤ J);  
 EXIT: THE SYMMETRIC DECOMPOSITION OF THE MATRIX IS  
 DELIVERED IN THE UPPER TRIANGLE OF A. THE SUPER-  
 DIAGONAL ELEMENTS OF THE UPPER-TRIANGULAR UNIT-  
 DIAGONAL MATRIX U ARE DELIVERED IN A[I,J], I < J;  
 THE DIAGONAL ELEMENTS OF THE DIAGONAL MATRIX ARE  
 DELIVERED IN A[I,I], I = 1, ..., N;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>; "ARRAY" AUX[2 : 3];  
 ENTRY:  
 AUX[2]: ENTRY: A RELATIVE TOLERANCE USED TO CONTROL THE  
 CALCULATION OF THE DIAGONAL ELEMENTS OF THE  
 DECOMPOSITION (AUX[2] > THE MACHINE PRECISION AND  
 AUX[2] > RELATIVE PRECISION OF THE MATRIX ELEMENTS,  
 SEE METHOD AND PERFORMANCE);  
 EXIT :  
 AUX[3] :  
 NORMAL EXIT: ABS(AUX[3]) = N;  
 AUX[3] = N, IF THE MATRIX IS (POSITIVE OR NEGATIVE)  
 DEFINITE;  
 AUX[3] = -N, IF THE DECOMPOSITION IS CARRIED OUT, BUT  
 THE MATRIX APPEARS TO BE NON-DEFINITE (SEE METHOD AND  
 PERFORMANCE);  
 FAILURE EXIT : 0 ≤ AUX[3] < N;  
 IF THE DECOMPOSITION CANNOT BE CARRIED OUT BECAUSE  
 SOME DIAGONAL ELEMENTS ARE TOO SMALL, AUX[3] = K - 1,  
 WHERE K IS THE LAST STAGE NUMBER OF THE DECOMPOSITION  
 (SEE METHOD AND PERFORMANCE).



PROCEDURES USED: TAMMAT ■ CP34014.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SYMDEC2 PERFORMS THE SYMMETRIC DECOMPOSITION OF A SYMMETRIC (POSITIVE OR NEGATIVE DEFINITE) MATRIX. THE METHOD USED IS  $U^T D U$  DECOMPOSITION WITHOUT PIVOTING (SEE REF [1], SECTION I / 1). IF THE GIVEN SYMMETRIC MATRIX IS DEFINITE, THE METHOD YIELDS AN UPPER-TRIANGULAR MATRIX WITH UNIT DIAGONAL AND A DIAGONAL MATRIX (ALL DIAGONAL ELEMENTS HAVING THE SAME SIGN) SUCH THAT  $U^T D U$  EQUALS THE GIVEN MATRIX. THE PROCESS IS TERMINATED AT STAGE K, IF THE ABSOLUTE VALUE OF THE K-TH DIAGONAL ELEMENT OF THE DIAGONAL MATRIX IS LESS THAN A TOLERANCE (AUX[2]) TIMES THE MAXIMAL ELEMENT OF THE GIVEN MATRIX. THIS TOLERANCE AUX[2] MUST BE CHOSEN LARGER THAN THE MACHINE PRECISION AND THE PRECISION OF THE ELEMENTS OF THE MATRIX. IF THE MATRIX CAN BE DECOMPOSED, BUT WITH DIAGONAL ELEMENTS HAVING DIFFERENT SIGNS (THE MATRIX IS NON-DEFINITE), THE SYMMETRIC DECOMPOSITION IS ALSO PERFORMED AND AUX[3] ASSUMES THE VALUE -N.

REFERENCES:

- [1]. J.H. WILKINSON AND C. REINSCH :  
HANDBOOK FOR AUTOMATIC COMPUTATION. VOL. 2. LINEAR ALGEBRA.  
SPRINGER VERLAG, BERLIN, (1971).

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF SYMINV2, SECTION 3.1.1.1.1.3.4.

SECTION : 3.1.1.1.1.3.1

(JANUARY 1976)

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SUBSECTION : SYMDEC1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" SYMDEC1(A, N, AUX); "VALUE" N; "INTEGER" N;  
 "ARRAY" A, AUX;  
 "CODE" 34701;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : (N + 1) \* N // 2];  
 ENTRY: THE UPPER-TRIANGULAR PART OF THE DEFINITE  
 SYMMETRIC MATRIX MUST BE GIVEN COLUMNWISE IN ARRAY A  
 (THE (I,J)-TH ELEMENT OF THE MATRIX MUST BE GIVEN IN  
 A[(J - 1) \* J // 2 + I] FOR 1 <= I <= J <= N);  
 EXIT: THE SYMMETRIC DECOMPOSITION OF THE MATRIX IS  
 DELIVERED COLUMNWISE IN A.

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>; "ARRAY" AUX[2 : 3];  
 AUX[2]: ENTRY: A RELATIVE TOLERANCE USED TO CONTROL THE  
 CALCULATION OF THE DIAGONAL ELEMENTS OF THE  
 DECOMPOSITION (AUX[2] > THE MACHINE PRECISION AND  
 AUX[2] > RELATIVE PRECISION OF THE MATRIX ELEMENTS,  
 SEE METHOD AND PERFORMANCE);  
 AUX[3] :  
 EXIT :  
 NORMAL EXIT: ABS(AUX[3]) = N;  
 AUX[3] = N, IF THE MATRIX IS (POSITIVE OR NEGATIVE)  
 DEFINITE;  
 AUX[3] = -N, IF THE DECOMPOSITION IS CARRIED OUT, BUT  
 THE MATRIX APPEARS TO BE NON-DEFINITE (SEE METHOD AND  
 PERFORMANCE);  
 FAILURE EXIT : 0 <= AUX[3] < N;  
 IF THE DECOMPOSITION CANNOT BE CARRIED OUT BECAUSE  
 SOME DIAGONAL ELEMENTS ARE TOO SMALL, AUX[3] = K - 1,  
 WHERE K IS THE LAST STAGE NUMBER OF THE DECOMPOSITION  
 (SEE METHOD AND PERFORMANCE).

PROCEDURES USED: VECVEC = CP34010.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

SECTION : 3.1.1.1.1.3.1

(JANUARY 1976)

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LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SYMDEC1 PERFORMS THE SYMMETRIC DECOMPOSITION OF A SYMMETRIC DEFINITE MATRIX, WHOSE UPPER TRIANGLE IS STORED IN A ONE-DIMENSIONAL ARRAY, BY PERFORMING THE  $U' D U =$  DECOMPOSITION. SEE ALSO METHOD AND PERFORMANCE OF SYMDEC2, (THIS SECTION).

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF SYMINV1, SECTION 3.1.1.1.1.3.4.

SOURCE TEXT(S) :

```

"CODE" 34700;
  "PROCEDURE" SYMDEC2(A, N, AUX); "VALUE" N; "INTEGER" N;
  "ARRAY" A, AUX;
  "BEGIN" "INTEGER" I, J; "REAL" W, H, R, EPSNORM;
    "REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B); "CODE" 34014;

    R := 0;
    "FOR" J := 1 "STEP" 1 "UNTIL" N "DO"
      "IF" ABS(A[J,J]) > R "THEN" R := ABS(A[J,J]);
    EPSNORM := AUX[2] * R; AUX[3] := N;
    "FOR" I := 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" "COMMENT" (* COLUMN WISE COMPUTATION OF U *);
        R := A[I,I]; "FOR" J := 1 "STEP" 1 "UNTIL" I - 1 "DO"
          "BEGIN" H := A[J,I]; W := A[J,I] / A[J,J]; R := R - H * W
        "END"
        (* D[I] := *); A[I,I] := R;
        "IF" SIGN(A[I,I]) = SIGN(R) "THEN" AUX[3] := - N;
        "IF" ABS(R) <= EPSNORM "THEN"
          "BEGIN" AUX[3] := I - 1; I := N "END" "ELSE"
          "FOR" J := I + 1 "STEP" 1 "UNTIL" N "DO"
            A[I,J] := A[I,J] - TAMMAT(1, I - 1, J, I, A, A);
          "COMMENT" (* = DU[I,J] *);
        "END" (* U' D U = DECOMPOSITION *)
      "END" SYMDEC2;
  "EOP"

```

```

"CODE" 34701;
"PROCEDURE" SYMDEC1(A, N, AUX); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX;
"BEGIN" "INTEGER" I, J, II, JJ, JI, LOW, UP; "REAL" R, EPSNORM, H, W;
"REAL" "PROCEDURE" VECVEC(L, U, SHIFT, A, B); "CODE" 34010;

R:= 0; II:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" II:= II + I; "IF" ABS(A[II]) > R "THEN" R:= ABS(A[II])
"END";
EPSNORM:= AUX[2] * R; AUX[3]:= N; II:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" LOW:= II + 1; II:= II + I; UP:= II - 1;
R:= A[II]; JJ:= J:= 0;
"FOR" JI:= LOW "STEP" 1 "UNTIL" UP "DO"
"BEGIN" J:= J + 1; JJ:= JJ + J; H:= A[JI];
W:= A[JI] := H / A[JJ]; R:= R * W
"END";
A[II] := R; "IF" SIGN(A[II]) = SIGN(R) "THEN" AUX[3] := N;
"IF" ABS(R) <= EPSNORM "THEN"
"BEGIN" AUX[3] := I - 1; I:= N "END" "ELSE"
"BEGIN" JI:= II + I; "FOR" J:= I + 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" A[JI] := A[JI] = VECVEC(LOW, UP, JI - II, A, A);
JI:= JI + J
"END"
"END"
"END"
"END" SYMDEC1;
"EOF"

```

SECTION : 3.1.1.1.1.3.2

(JANUARY 1976)

PAGE 1

CONTRIBUTOR : J. KOK.

INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED:

BRIEF DESCRIPTION:

THIS SECTION CONTAINS TWO PROCEDURES:

- A) SYMDETERM2 CALCULATES THE DETERMINANT OF A SYMMETRIC (DEFINITE) MATRIX IF THE SYMMETRIC DECOMPOSITION IS PERFORMED BY SYMDEC2;
- B) SYMDETERM1 CALCULATES THE DETERMINANT OF A SYMMETRIC (DEFINITE) MATRIX IF THE SYMMETRIC DECOMPOSITION IS PERFORMED BY SYMDEC1.

KEYWORDS:

DETERMINANT,  
DEFINITE SYMMETRIC MATRIX.

SUBSECTION: SYMDETERM2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"REAL" "PROCEDURE" SYMDETERM2(A, N); "VALUE" N; "INTEGER" N;  
"ARRAY" A;  
"CODE" 34702;

SYMDETERM2 DELIVERS THE DETERMINANT OF THE SYMMETRIC DEFINITE MATRIX WHICH HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF SYMDEC2;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : N, 1 : N];  
ENTRY: THE RESULTS OF THE U' D U = DECOMPOSITION AS PERFORMED BY SYMDEC2 (SECTION 3.1.1.1.1.3.1) OR SYMDECSOL2 (SECTION 3.1.1.1.1.3.3) SHOULD BE GIVEN IN THE UPPER TRIANGLE OF A;  
EXIT: THE CONTENTS OF A ARE NOT CHANGED;  
N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE MATRIX.

SECTION : 3.1.1.1.1.3.2

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PROCEDURES USED :

DETERM = CP34303.

RUNNING TIME: PROPORTIONAL TO N.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE SYMDETERM2 SHOULD BE CALLED AFTER A SUCCESSFUL CALL OF SYMDEC2 OR SYMDECSOL2, I.E. IF  $ABS(AUX[3]) \neq N$ .

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF SYMDECINV2, SECTION 3.1.1.1.1.3.4.

SUBSECTION: SYMDETERM1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
"REAL" "PROCEDURE" SYMDETERM1(A, N); "VALUE" N; "INTEGER" N;  
"ARRAY" A;  
"CODE" 34703;

SYMDETERM1 DELIVERS THE DETERMINANT OF THE SYMMETRIC DEFINITE MATRIX WHICH HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF SYMDEC1.

THE MEANING OF THE FORMAL PARAMETERS IS:  
A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : (N + 1) \* N // 2];  
ENTRY: THE RESULTS OF THE U<sup>T</sup> D U = DECOMPOSITION AS PERFORMED BY SYMDEC1 (SECTION 3.1.1.1.1.3.1) OR SYMDECSOL1 (SECTION 3.1.1.1.1.3.3) SHOULD BE GIVEN IN ARRAY A;  
EXIT: THE CONTENTS OF A ARE NOT CHANGED;  
N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE MATRIX.

PROCEDURES USED :

GIANT = CP30004,  
OVERFLOW = CP30008.

RUNNING TIME: PROPORTIONAL TO N.

SECTION : 3.1.1.1.1.3.2

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LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE SYMDETERM1 SHOULD BE CALLED AFTER A SUCCESSFUL CALL OF SYMDEC1 OR SYMDECSOL1, I.E. IF  $ABS(AUX[3]) = N$ .

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF SYMDECINV1, SECTION 3.1.1.1.1.3.4.

SOURCE TEXT(S) :

```
"CODE" 34702;
  "REAL" "PROCEDURE" SYMDETERM2(A, N); "VALUE" N; "INTEGER" N;
  "ARRAY" A;
  "BEGIN" "INTEGER" K, D;
    "REAL" "PROCEDURE" DETERM(A, N, SGN); "CODE" 34303;
    D := 1;
    "FOR" K := 1 "STEP" 1 "UNTIL" N "DO"
      "IF" A[K,K] < 0 "THEN" D := - D;
    SYMDETERM2 := DETERM(A, N, D)
  "END" SYMDETERM2;
  "EOP"
```

```
"CODE" 34703;
  "REAL" "PROCEDURE" SYMDETERM1(A, N); "VALUE" N; "INTEGER" N;
  "ARRAY" A;
  "BEGIN" "INTEGER" K, KK, S; "REAL" D;
    "REAL" "PROCEDURE" GIANT; "CODE" 30004;
    "BOOLEAN" "PROCEDURE" OVERFLOW(X); "CODE" 30008;
    S := 1; KK := 0;
    "FOR" K := 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" KK := KK + K; "IF" A[KK] < 0 "THEN" S := - S "END";
    D := 1; KK := 0;
    "FOR" K := 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" KK := KK + K; D := A[KK] * D; "IF" OVERFLOW(D) "THEN"
        "BEGIN" D := GIANT * S; K := N "END"
      "END";
    SYMDETERM1 := D
  "END" SYMDETERM1;
  "EOP"
```

SECTION : 3.1.1.1.1.3.3

(JANUARY 1976)

PAGE 1

AUTHOR: J. KOK.

INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED :

BRIEF DESCRIPTION:

THIS SECTION CONTAINS FOUR PROCEDURES:

- A) SYMSOL2 CALCULATES THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS IF THE COEFFICIENT MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE SYMDEC2, SECTION 3.1.1.1.1.3.1., OR SYMDECSOL2;
- B) SYMSOL1 CALCULATES THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS IF THE COEFFICIENT MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE SYMDEC1, SECTION 3.1.1.1.1.3.1., OR SYMDECSOL1;
- C) SYMDECSOL2 CALCULATES THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS. THE COEFFICIENT MATRIX HAS TO BE SYMMETRIC AND MUST BE GIVEN IN THE UPPER TRIANGLE OF A TWO-DIMENSIONAL ARRAY;
- D) SYMDECSOL1 CALCULATES THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS. THE COEFFICIENT MATRIX HAS TO BE SYMMETRIC AND MUST BE GIVEN COLUMNWISE IN A ONE-DIMENSIONAL ARRAY.

KEYWORDS:

LINEAR EQUATIONS,  
DEFINITE SYMMETRIC MATRIX,  
SYMMETRIC DECOMPOSITION.



## SUBSECTION: SYMSOL2.

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" SYMSOL2(A, N, B); "VALUE" N; "INTEGER" N; "ARRAY" A, B;  
 "CODE" 34704;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : N, 1 : N];  
 ENTRY: THE RESULTS OF THE DECOMPOSITION OF THE GIVEN MATRIX  
 AS PRODUCED BY SYMDEC2, SECTION 3.1.1.1.1.3.1., OR  
 SYMDECSOL2 (THIS SECTION), SHOULD BE GIVEN IN THE  
 ARRAY A;  
 EXIT: THE ELEMENTS OF A ARE NOT CHANGED;  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;  
 B: <ARRAY IDENTIFIER>; "ARRAY" B[1 : N];  
 ENTRY: THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR  
 EQUATIONS;  
 EXIT: THE SOLUTION OF THE SYSTEM.

## PROCEDURES USED:

MATVEC = CP34011,  
 TAMVEC = CP34012.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N SQUARED.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

THE PROCEDURE SYMSOL2 CALCULATES THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS, PROVIDED THAT THE COEFFICIENT MATRIX HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF SYMDEC2 OR SYMDECSOL2;  
 THE SOLUTION IS OBTAINED BY PERFORMING THE FORWARD AND BACKWARD SUBSTITUTIONS.  
 THE RIGHT HAND SIDE IS OVERWRITTEN BY THE SOLUTION BUT THE CONTENTS OF THE MATRIX STORAGE ARRAY ARE NOT CHANGED, THUS SEVERAL SYSTEMS OF LINEAR EQUATIONS WITH THE SAME COEFFICIENT MATRIX BUT DIFFERENT RIGHT HAND SIDES CAN BE SOLVED BY SUCCESSIVE CALLS OF SYMSOL2.

## EXAMPLE OF USE:

SEE EXAMPLE OF USE OF SYMINV2, SECTION 3.1.1.1.1.3.4.

SUBSECTION: SYMSOL1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
"PROCEDURE" SYMSOL1(A, N, B); "VALUE" N; "INTEGER" N; "ARRAY" A, B;  
"CODE" 34705;

THE MEANING OF THE FORMAL PARAMETERS IS:  
A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : (N + 1) \* N // 2];  
ENTRY: THE RESULTS OF THE DECOMPOSITION OF THE GIVEN MATRIX  
AS PRODUCED BY SYMDEC1, SECTION 3.1.1.1.1.3.1., OR  
SYMDECSOL1 (THIS SECTION), MUST BE GIVEN IN ARRAY  
A;  
EXIT: THE ELEMENTS OF A ARE NOT CHANGED;  
N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE MATRIX;  
B: <ARRAY IDENTIFIER>; "ARRAY" B[1 : N];  
ENTRY: THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR  
EQUATIONS;  
EXIT: THE SOLUTION OF THE SYSTEM.

PROCEDURES USED:

VECVEC = CP34010,  
"CODE" 34710;  
SEQVEC = CP34016.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N SQUARED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE SYMSOL1 CALCULATES THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS, PROVIDED THAT THE COEFFICIENT MATRIX HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF SYMDEC1 OR SYMDECSOL1; SEVERAL SYSTEMS WITH THE SAME COEFFICIENT MATRIX BUT DIFFERENT RIGHT HAND SIDES CAN BE SOLVED BY SUCCESSIVE CALLS OF SYMSOL1. SEE ALSO METHOD AND PERFORMANCE OF SYMSOL2 (THIS SECTION).

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF SYMINV1, SECTION 3.1.1.1.1.3.4.

SECTION : 3.1.1.1.1.3.3

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SUBSECTION: SYMDECSOL2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" SYMDECSOL2(A, N, AUX, B); "VALUE" N; "INTEGER" N;  
 "ARRAY" A, AUX, B;  
 "CODE" 347067

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : N, 1 : N];  
 ENTRY: THE UPPER TRIANGLE OF THE DEFINITE SYMMETRIC MATRIX  
 MUST BE GIVEN IN THE UPPER-TRIANGULAR PART OF A (THE  
 ELEMENTS A[I,J], I <= J);  
 EXIT: THE SYMMETRIC DECOMPOSITION OF THE MATRIX IS  
 DELIVERED IN THE UPPER TRIANGLE OF A. THE SUPER-  
 DIAGONAL ELEMENTS OF THE UPPER-TRIANGULAR UNIT-  
 DIAGONAL MATRIX U ARE DELIVERED IN A[I,J], I < J;  
 THE DIAGONAL ELEMENTS OF THE DIAGONAL MATRIX ARE  
 DELIVERED IN A[I,I], I = 1, ..., N;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>; "ARRAY" AUX[2 : 3];  
 AUX[2]: ENTRY: A RELATIVE TOLERANCE USED TO CONTROL THE  
 CALCULATION OF THE DIAGONAL ELEMENTS OF THE  
 DECOMPOSITION (AUX[2] > THE MACHINE PRECISION AND  
 AUX[2] > RELATIVE PRECISION OF THE MATRIX ELEMENTS,  
 SEE METHOD AND PERFORMANCE);  
 AUX[3] :  
 EXIT :  
 NORMAL EXIT (ABS(AUX[3]) = N) : THE SOLUTION IS DELIVERED;  
 AUX[3] = N, IF THE MATRIX IS (POSITIVE OR NEGATIVE)  
 DEFINITE;  
 AUX[3] = -N, IF THE DECOMPOSITION IS CARRIED OUT, BUT  
 THE MATRIX APPEARS TO BE NON-DEFINITE (SEE METHOD AND  
 PERFORMANCE);  
 FAILURE EXIT (0 <= AUX[3] < N) : NO SOLUTION IS DELIVERED;  
 IF THE DECOMPOSITION CANNOT BE CARRIED OUT BECAUSE  
 SOME DIAGONAL ELEMENTS ARE TOO SMALL, AUX[3] = K = 1,  
 WHERE K IS THE LAST STAGE NUMBER OF THE DECOMPOSITION  
 (SEE METHOD AND PERFORMANCE);

B: <ARRAY IDENTIFIER>; "ARRAY" B[1 : N];  
 ENTRY: THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR  
 EQUATIONS;  
 EXIT: THE SOLUTION OF THE SYSTEM.

PROCEDURES USED:

SYMDEC2 = CP34700,

SYMSOL2 = CP34704.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

SECTION : 3.1.1.1.1.3.3

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## METHOD AND PERFORMANCE:

THE PROCEDURE SYMDECSOL2 SOLVES A SYSTEM OF LINEAR EQUATIONS WITH A SYMMETRIC DEFINITE COEFFICIENT MATRIX BY CALLING SYMDEC2, SECTION 3.1.1.1.1.3.1., AND, IF THIS CALL WAS SUCCESSFUL, SYMSOL2 (THIS SECTION).  
SEE ALSO SYMDEC2, SECTION 3.1.1.1.1.3.1.

EXAMPLE OF USE: SEE EXAMPLE OF USE OF SYMDECINV2, SECTION 3.1.1.1.1.3.4

SUBSECTION: SYMDECSOL1.

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
"PROCEDURE" SYMDECSOL1(A, N, AUX, B); "VALUE" N; "INTEGER" N;  
"ARRAY" A, AUX, B;  
"CODE" 34707;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : (N + 1) \* N // 2];  
ENTRY: THE UPPER-TRIANGULAR PART OF THE (DEFINITE) SYMMETRIC MATRIX MUST BE GIVEN COLUMNWISE IN ARRAY A (THE (I,J)-TH ELEMENT OF THE MATRIX MUST BE GIVEN IN A[(J - 1) \* J // 2 + I] FOR 1 <= I <= J <= N);  
EXIT: THE RESULTS OF THE U' D U = DECOMPOSITION OF THE MATRIX ARE DELIVERED IN THIS ARRAY;

N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>; "ARRAY" AUX[2 : 3];  
AUX[2]: ENTRY: A RELATIVE TOLERANCE USED TO CONTROL THE CALCULATION OF THE DIAGONAL ELEMENTS OF THE DECOMPOSITION (AUX[2] > THE MACHINE PRECISION AND AUX[2] > RELATIVE PRECISION OF THE MATRIX ELEMENTS, SEE METHOD AND PERFORMANCE);  
AUX[3] :  
EXIT :  
NORMAL EXIT (ABS(AUX[3]) = N) : THE SOLUTION IS DELIVERED;  
AUX[3] = N, IF THE MATRIX IS (POSITIVE OR NEGATIVE) DEFINITE;  
AUX[3] = -N, IF THE DECOMPOSITION IS CARRIED OUT, BUT THE MATRIX APPEARS TO BE NON-DEFINITE (SEE METHOD AND PERFORMANCE);  
FAILURE EXIT (0 <= AUX[3] < N) : NO SOLUTION IS DELIVERED;  
IF THE DECOMPOSITION CANNOT BE CARRIED OUT BECAUSE SOME DIAGONAL ELEMENTS ARE TOO SMALL, AUX[3] = K - 1, WHERE K IS THE LAST STAGE NUMBER OF THE DECOMPOSITION (SEE METHOD AND PERFORMANCE);

B: <ARRAY IDENTIFIER>; "ARRAY" B[1 : N];  
ENTRY: THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR EQUATIONS;  
EXIT: THE SOLUTION OF THE SYSTEM.

SECTION : 3.1.1.1.1.3.3

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## PROCEDURES USED:

SYMDEC1 = CP 34701,  
 SYMSOL1 = CP 34705.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

THE PROCEDURE SYMDECSOL1 SOLVES A SYSTEM OF LINEAR EQUATIONS WITH A SYMMETRIC DEFINITE COEFFICIENT MATRIX BY CALLING SYMDEC1, SECTION 3.1.1.1.1.3.1., AND, IF THIS CALL WAS SUCCESSFUL, SYMSOL1 (THIS SECTION). THE UPPER TRIANGLE OF THE COEFFICIENT MATRIX SHOULD BE STORED COLUMN-WISE IN A ONE-DIMENSIONAL ARRAY. SEE ALSO SYMDEC2, SECTION 3.1.1.1.1.3.1.

## EXAMPLE OF USE:

SEE EXAMPLE OF USE OF SYMDECINV1, SECTION 3.1.1.1.1.3.4.

## SOURCE TEXT(S) :

```
"CODE" 34704;
  "PROCEDURE" SYMSOL2(A, N, B); "VALUE" N; "INTEGER" N; "ARRAY" A, B;
  "BEGIN" "INTEGER" I;
    "REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
    "REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;

    "COMMENT" (* U' Y = B *);
    "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
      R[I]:= B[I] = TAMVEC(1, I = 1, I, A, B);
    "COMMENT" (* D U X = Y *);
    "FOR" I:= N "STEP" = 1 "UNTIL" 1 "DO"
      R[I]:= B[I] / A[I, I] = MATVEC(I + 1, N, I, A, B)
  "END" SYMSOL2;
  "EOP"
```

```

"CODE" 34705;
"PROCEDURE" SYMSOL1(A, N, B); "VALUE" N; "INTEGER" N; "ARRAY" A, B;
"BEGIN" "INTEGER" I, II;
"REAL" "PROCEDURE" VECVEC(L, U, SHIFT, A, B); "CODE" 34010;
"REAL" "PROCEDURE" SEQVEC(L, U, I1, SHIFT, A, B); "CODE" 34016;

II:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" II:= II + I;
      B[II]:= B[I] - VECVEC(1, I - 1, II - I, B, A)
"END";
"FOR" I:= N "STEP" - 1 "UNTIL" 1 "DO"
"BEGIN" B[II]:= B[I] / A[II] - SEQVEC(I + 1, N, II + I, 0, A,
      B); II:= II - I
"END"
"END" SYMSOL1;
"EOP"

```

```

"CODE" 34706;
"PROCEDURE" SYMDECSOL2(A, N, AUX, B); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX, B;
"BEGIN"
"PROCEDURE" SYMDEC2(A, N, AUX); "CODE" 34700;
"PROCEDURE" SYMSOL2(A, N, B); "CODE" 34704;

SYMDEC2(A, N, AUX);
"IF" ABS(AUX[3]) = N "THEN" SYMSOL2(A, N, B)
"END" SYMDECSOL2;
"EOP"

```

```

"CODE" 34707;
"PROCEDURE" SYMDECSOL1(A, N, AUX, B); "VALUE" N; "INTEGER" N;
"ARRAY" A, AUX, B;
"BEGIN"
"PROCEDURE" SYMDEC1(A, N, AUX); "CODE" 34701;
"PROCEDURE" SYMSOL1(A, N, B); "CODE" 34705;

SYMDEC1(A, N, AUX);
"IF" ABS(AUX[3]) = N "THEN" SYMSOL1(A, N, B)
"END" SYMDECSOL1;
"EOP"

```

SECTION : 3.1.1.1.1.3.4

(JANUARY 1976)

PAGE 1

AUTHOR : J. KOK.

INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED : 751215.

**BRIEF DESCRIPTION:**

THIS SECTION CONTAINS FOUR PROCEDURES:

- A) SYMINV2 CALCULATES THE INVERSE OF A SYMMETRIC MATRIX, IF THE MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE SYMDEC2, SECTION 3.1.1.1.1.3.1., OR SYMDECSOL2, SECTION 3.1.1.1.1.3.3.;
- B) SYMINV1 CALCULATES THE INVERSE OF A SYMMETRIC MATRIX, IF THE MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE SYMDEC1, SECTION 3.1.1.1.1.3.1., OR SYMDECSOL1, SECTION 3.1.1.1.1.3.3.;
- C) SYMDECINV2 CALCULATES THE INVERSE OF A MATRIX USING SYMMETRIC DECOMPOSITION, THE COEFFICIENT MATRIX HAS TO BE SYMMETRIC AND MUST BE GIVEN IN THE UPPER TRIANGLE OF A TWO-DIMENSIONAL ARRAY;
- D) SYMDECINV1 CALCULATES THE INVERSE OF A MATRIX USING SYMMETRIC DECOMPOSITION, THE COEFFICIENT MATRIX HAS TO BE SYMMETRIC AND MUST BE GIVEN COLUMNWISE IN A ONE-DIMENSIONAL ARRAY.

**KEYWORDS:**

MATRIX INVERSION,  
DEFINITE SYMMETRIC MATRIX,  
SYMMETRIC DECOMPOSITION.

SECTION : 3.1.1.1.1.3.4 (JANUARY 1976)

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SUBSECTION: SYMINV2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" SYMINV2(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;  
 "CODE" 34708;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : N, 1 : N];  
 ENTRY: THE RESULTS OF THE DECOMPOSITION OF THE GIVEN MATRIX  
 AS PRODUCED BY SYMDEC2, SECTION 3.1.1.1.1.3.1., OR  
 SYMDECSOL2, SECTION 3.1.1.1.1.3.3., MUST BE GIVEN  
 IN THE UPPER TRIANGLE OF A;  
 EXIT: THE UPPER-TRIANGULAR PART OF THE INVERSE MATRIX IS  
 DELIVERED IN THE UPPER TRIANGLE OF A;  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX.

PROCEDURES USED:

MATVEC = CP34011,  
 TAMVEC = CP34012,  
 DUPVECROW = CP31031.

REQUIRED CENTRAL MEMORY:

AN ARRAY OF N REALS IS DECLARED.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE SYMINV2 CALCULATES THE INVERSE OF A MATRIX, PROVIDED  
 THAT THE MATRIX HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF SYMDEC2  
 OR SYMDECSOL2;  
 THE INVERSE, X, OF U'DU, WHERE U AND D ARE THE RESULTS OF THE  
 DECOMPOSITION,  
 IS OBTAINED FROM THE CONDITIONS THAT X IS SYMMETRIC AND DUX IS  
 A LOWER-TRIANGULAR MATRIX WITH UNIT DIAGONAL ELEMENTS. THE UPPER-  
 TRIANGULAR ELEMENTS OF X ARE CALCULATED BY BACK SUBSTITUTION.  
 THE UPPER TRIANGLE OF THE INVERSE MATRIX IS DELIVERED IN THE UPPER  
 TRIANGLE OF THE GIVEN ARRAY.



## EXAMPLE OF USE:

THE UPPER TRIANGLE OF THE SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX (THE PASCAL MATRIX OF ORDER 4) OF THE SYSTEM OF EQUATIONS

$$\begin{array}{r}
 X_1 + \quad \quad X_2 + \quad \quad \quad X_3 + \quad \quad \quad X_4 = 2 \\
 X_1 + 2 * X_2 + \quad 3 * X_3 + \quad 4 * X_4 = 4 \\
 X_1 + 3 * X_2 + \quad 6 * X_3 + 10 * X_4 = 8 \\
 X_1 + 4 * X_2 + 10 * X_3 + 20 * X_4 = 16
 \end{array}$$

IS STORED IN THE TWO-DIMENSIONAL ARRAY PASCAL2. THE INVERSE OF THE COEFFICIENT MATRIX AND THE SOLUTION OF THE LINEAR SYSTEM ARE CALCULATED BY THE FOLLOWING PROGRAM:

```

"BEGIN" "COMMENT" TEST SYMDEC2, SYMSOL2 AND SYMINV2;
  "INTEGER" I, J;
  "ARRAY" PASCAL2[1:4,1:4], B[1:4], AUX[2:3];

  "PROCEDURE" SYMDEC2(A, N, AUX); "CODE" 34700;
  "PROCEDURE" SYMSOL2(A, N, B); "CODE" 34704;
  "PROCEDURE" SYMINV2(A, N); "CODE" 34708;

  "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" PASCAL2[1,J]:= 1;
    "FOR" I:= 2 "STEP" 1 "UNTIL" J "DO"
    PASCAL2[I,J]:= "IF" I = J "THEN" PASCAL2[I-1,J] * 2 "ELSE"
      PASCAL2[I,J-1] + PASCAL2[I-1,J];
    B[J]:= 2 ** J
  "END";

  AUX[2]:= "-11;
  SYMDEC2(PASCAL2, 4, AUX);
  "IF" AUX[3] < 4 "THEN"
    OUTPUT(61, "("("MATRIX NOT DEFINITE"), "/)") "ELSE"
  "BEGIN" SYMSOL2(PASCAL2, 4, B); SYMINV2(PASCAL2, 4);
    OUTPUT(61, "("4B, "("SOLUTION USING SYMDEC2 ")",
      "("AND SYMSOL2:", "/)");
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
    OUTPUT(61, "("4B+D.5D)", B[I]);
    OUTPUT(61, "("//, 4B,
      "("INVERSE MATRIX USING SYMINV2:", /, 4B)");
    "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
    "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
      "IF" J < I "THEN" OUTPUT(61, "("12B)") "ELSE"
      OUTPUT(61, "("+ZD.5D3B)", PASCAL2[I,J]);
      OUTPUT(61, "("/, 4B)")
    "END"
  "END"
"END"
"END"

```

SECTION : 3.1.1.1.1.3.4

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THIS PROGRAM DELIVERS:

SOLUTION USING SYMDEC2 AND SYMSOL2:

+0.00000      +4.00000      -4.00000      +2.00000

INVERSE MATRIX USING SYMINV2:

+4.00000	-6.00000	+4.00000	-1.00000
	+14.00000	-11.00000	+3.00000
		+10.00000	-3.00000
			+1.00000

SUBSECTION: SYMINV1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"PROCEDURE" SYMINV1(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;  
 "CODE" 34709;

THE MEANING OF THE FORMAL PARAMETERS IS:

A:      <ARRAY IDENTIFIER>; "ARRAY" A[1 : (N + 1) \* N // 2];  
 ENTRY: THE RESULTS OF THE DECOMPOSITION OF THE GIVEN MATRIX  
 AS PRODUCED BY SYMDEC1, SECTION 3.1.1.1.1.3.1., OR  
 SYMDECSOL1, SECTION 3.1.1.1.1.3.3., MUST BE GIVEN  
 IN ARRAY A;  
 EXIT: THE UPPER-TRIANGULAR PART OF THE INVERSE MATRIX IS  
 DELIVERED COLUMNWISE IN ARRAY A;  
 N:      <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX.

PROCEDURES USED:

SE3VEC      = CP34016,  
 SYMMATVEC = CP34018.

REQUIRED CENTRAL MEMORY:

AN ARRAY OF N REALS IS DECLARED.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

THE PROCEDURE SYMINV1 CALCULATES THE INVERSE OF A MATRIX, PROVIDED THAT THE MATRIX HAS BEEN DECOMPOSED BY A SUCCESSFUL CALL OF SYMDEC1 OR SYMDECSOL1;  
THE UPPER TRIANGLE OF THE INVERSE MATRIX IS DELIVERED COLUMNWISE IN THE ONE-DIMENSIONAL ARRAY.  
SEE ALSO METHOD AND PERFORMANCE OF SYMINV2 (THIS SECTION).

## EXAMPLE OF USE:

THE UPPER TRIANGLE OF THE SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX (THE PASCAL MATRIX OF ORDER 4) OF THE SYSTEM OF EQUATIONS

$$\begin{array}{rcl}
 x_1 + & x_2 + & x_3 + & x_4 = & 2 \\
 x_1 + 2 * & x_2 + & 3 * & x_3 + & 4 * & x_4 = & 4 \\
 x_1 + 3 * & x_2 + & 6 * & x_3 + & 10 * & x_4 = & 8 \\
 x_1 + 4 * & x_2 + & 10 * & x_3 + & 20 * & x_4 = & 16
 \end{array}$$

IS STORED IN THE ONE-DIMENSIONAL ARRAY PASCAL1.  
THE INVERSE OF THE COEFFICIENT MATRIX AND THE SOLUTION OF THE LINEAR SYSTEM ARE CALCULATED BY THE FOLLOWING PROGRAM:

```

"BEGIN" "COMMENT" TEST SYMDEC1, SYMSOL1 AND SYMINV1;
  "INTEGER" I, J, JJ;
  "ARRAY" PASCAL1[1:(4 + 1) * 4 // 2], B[1:4], AUX[2:3];

  "PROCEDURE" SYMDEC1(A, N, AUX); "CODE" 34701;
  "PROCEDURE" SYMSOL1(A, N, B); "CODE" 34705;
  "PROCEDURE" SYMINV1(A, N); "CODE" 34709;

  JJ:= 1;
  "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" PASCAL1[JJ]:= 1;
    "FOR" I:= 2 "STEP" 1 "UNTIL" J "DO"
    PASCAL1[JJ + I - 1]:= "IF" I = J "THEN"
    PASCAL1[JJ + I - 2] * 2 "ELSE"
    PASCAL1[JJ + I - 2] + PASCAL1[JJ + I - J];
    B[J]:= 2 ** J;
    JJ:= JJ + J
  "END";

```

```

AUX[2] := "-11";
SYMDEC1(PASCAL1, 4, AUX);
"IF" AUX[3] < 4 "THEN"
  OUTPUT(61, "("("MATRIX NOT DEFINITE")", /)") "ELSE"
"BEGIN" SYMSOL1(PASCAL1, 4, B); SYMINV1(PASCAL1, 4);
  OUTPUT(61, "("4B,
    "("SOLUTION USING SYMDEC1 AND SYMSOL1:"")", /)");
  "FOR" I := 1 "STEP" 1 "UNTIL" 4 "DO"
  OUTPUT(61, "("4B+D.5D")", B[I]);
  OUTPUT(61, "("2/, 4B,
    "("INVERSE MATRIX USING SYMINV1:"")", /, 4B)");
  "FOR" I := 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J := 1 "STEP" 1 "UNTIL" 4 "DO"
    "IF" J < I "THEN" OUTPUT(61, "("12B)") "ELSE"
    OUTPUT(61, "("+ZD.5D3B")", PASCAL1[(J - 1) * J // 2 + I]);
    OUTPUT(61, "("/, 4B)")
  "END"
"END"
"END"
"END"

```

## THIS PROGRAM DELIVERS:

## SOLUTION USING SYMDEC1 AND SYMSOL1:

+0.00000	+4.00000	-4.00000	+2.00000
----------	----------	----------	----------

## INVERSE MATRIX USING SYMINV1:

+4.00000	-6.00000	+4.00000	=1.00000
	+14.00000	-11.00000	+3.00000
		+10.00000	=3.00000
			+1.00000

SECTION : 3.1.1.1.1.3.4

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SUBSECTION: SYMDECINV2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" SYMDECINV2(A, N, AUX); "VALUE" N; "INTEGER" N;  
 "ARRAY" A, AUX;  
 "CODE" 347101

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : N, 1 : N];  
 ENTRY: THE UPPER TRIANGLE OF THE SYMMETRIC MATRIX  
 MUST BE GIVEN IN THE UPPER TRIANGLE OF A (THE  
 ELEMENTS A[I,J], I <= J);  
 EXIT: THE UPPER-TRIANGULAR PART OF THE INVERSE MATRIX IS  
 DELIVERED IN THE UPPER TRIANGLE OF A.

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>; "ARRAY" AUX[2 : 3];  
 AUX[2]: ENTRY: A RELATIVE TOLERANCE USED TO CONTROL THE  
 CALCULATION OF THE DIAGONAL ELEMENTS OF THE  
 DECOMPOSITION (AUX[2] > THE MACHINE PRECISION AND  
 AUX[2] > RELATIVE PRECISION OF THE MATRIX ELEMENTS,  
 SEE METHOD AND PERFORMANCE);

AUX[3] :  
 EXIT :  
 NORMAL EXIT: ABS(AUX[3]) = N;  
 AUX[3] = N, IF THE MATRIX IS (POSITIVE OR NEGATIVE)  
 DEFINITE;  
 AUX[3] = -N, IF THE INVERSION IS CARRIED OUT, BUT  
 THE MATRIX APPEARS TO BE NON-DEFINITE (SEE METHOD AND  
 PERFORMANCE);  
 FAILURE EXIT : 0 <= AUX[3] < N;  
 IF THE INVERSION CANNOT BE CARRIED OUT BECAUSE SOME  
 DIAGONAL ELEMENTS OF THE DECOMPOSITION ARE TOO SMALL,  
 AUX[3] = K-1, WHERE K IS THE LAST STAGE NUMBER OF THE  
 DECOMPOSITION (SEE METHOD AND PERFORMANCE).

PROCEDURES USED:

SYMDEC2 = CP34700,  
 SYMINV2 = CP34708.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

THE PROCEDURE SYMDECINV2 CALCULATES THE INVERSE OF A SYMMETRIC DEFINITE MATRIX BY CALLING SYMDEC2 AND, IF THIS CALL WAS SUCCESSFUL, SYMINV2.

THE UPPER TRIANGLE OF THE INVERSE MATRIX IS DELIVERED IN THE UPPER TRIANGLE OF THE GIVEN ARRAY.

SEE ALSO METHOD AND PERFORMANCE OF SYMINV2 (THIS SECTION) AND SYMDEC2, SECTION 3.1.1.1.1.3.1.

## EXAMPLE OF USE:

THE UPPER TRIANGLE OF THE SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX (THE PASCAL MATRIX OF ORDER 4) OF THE SYSTEM OF EQUATIONS

$$\begin{array}{r}
 x_1 + \quad \quad x_2 + \quad \quad \quad x_3 + \quad \quad \quad x_4 = 2 \\
 x_1 + 2 * x_2 + \quad \quad 3 * x_3 + \quad \quad 4 * x_4 = 4 \\
 x_1 + 3 * x_2 + \quad \quad 6 * x_3 + \quad \quad 10 * x_4 = 8 \\
 x_1 + 4 * x_2 + \quad \quad 10 * x_3 + \quad \quad 20 * x_4 = 16
 \end{array}$$

IS STORED IN THE TWO-DIMENSIONAL ARRAY PASCAL2. THE DETERMINANT AND THE INVERSE OF THE COEFFICIENT MATRIX AND THE SOLUTION OF THE LINEAR SYSTEM ARE CALCULATED BY THE FOLLOWING PROGRAM:

```

"BEGIN" "COMMENT" TEST SYMDECSOL2, SYMDETERM2 AND SYMDECINV2;
"INTEGER" I, J;
"ARRAY" PASCAL2[1:4,1:4], B[1:4], AUX[2:3];
"REAL" DETERMINANT;

"PROCEDURE" SYMDECSOL2(A, N, AUX, B); "CODE" 34706;
"REAL" "PROCEDURE" SYMDETERM2(A, N); "CODE" 34702;
"PROCEDURE" SYMDECINV2(A, N, AUX); "CODE" 34710;

"PROCEDURE" FILLPASCAL(N); "VALUE" N; "INTEGER" N;
"BEGIN" "INTEGER" I, J;
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" PASCAL2[I,J]:= 1;
"FOR" I:= 2 "STEP" 1 "UNTIL" J "DO"
PASCAL2[I,J]:= "IF" I = J "THEN" PASCAL2[I-1,J] * 2
"ELSE" PASCAL2[I,J-1] + PASCAL2[I-1,J];
B[J]:= 2 ** J
"END"
"END" FILL PASCAL;

```

```

AUX[2]:= "-11; FILLPASCAL(4);
SYMDECSOL2(PASCAL2, 4, AUX, B);
"IF" AUX[3] < 4 "THEN"
OUTPUT(61, "("("MATRIX NOT POSITIVE DEFINITE")", /")") "ELSE"
"BEGIN" DETERMINANT:= SYMDETERM2(PASCAL2, 4);
  OUTPUT(61, "("4B")");
  OUTPUT(61, "("("SOLUTION USING SYMDECSOL2:")", /")");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  OUTPUT(61, "("4B+D.5D")", B[I]);
  OUTPUT(61, "("//, 4B, "("DETERMINANT USING SYMDETERM2: ")",
    +D.5D, 2/, 4B")", DETERMINANT);

  FILLPASCAL(4);
  SYMDECINV2(PASCAL2, 4, AUX);

  OUTPUT(61, "("("INVERSE MATRIX USING SYMDECINV2:")", /,
    4B")");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    "IF" J < I "THEN" OUTPUT(61, "("12B")") "ELSE"
    OUTPUT(61, "("+2D.5D3B")", PASCAL2[I,J]);
    OUTPUT(61, "("//, 4B")")
  "END"
"END"
"END"
"END"

```

THIS PROGRAM DELIVERS:

SOLUTION USING SYMDECSOL2:

+0.00000      +4.00000      -4.00000      +2.00000

DETERMINANT USING SYMDETERM2: +1.00000

INVERSE MATRIX USING SYMDECINV2:

+4.00000	-6.00000	+4.00000	-1.00000
	+14.00000	-11.00000	+3.00000
		+10.00000	-3.00000
			+1.00000

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SUBSECTION: SYMDECI V1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" SYMDECINV1(A, N, AUX); "VALUE" N; "INTEGER" N;  
 "CODE" 34711;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>; "ARRAY" A[1 : (N+1) \* N // 2];  
 ENTRY: THE UPPER-TRIANGULAR PART OF THE SYMMETRIC MATRIX  
 MUST BE GIVEN COLUMNWISE IN ARRAY A  
 (THE (I,J)-TH ELEMENT OF THE MATRIX MUST BE GIVEN IN  
 A[(J - 1) \* J // 2 + I] FOR 1 <= I <= J <= N);  
 EXIT: THE UPPER-TRIANGULAR PART OF THE INVERSE MATRIX IS  
 DELIVERED COLUMNWISE IN ARRAY A;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX:  
 <ARRAY IDENTIFIER>; "ARRAY" AUX[2 : 3];  
 AUX[2]: ENTRY: A RELATIVE TOLERANCE USED TO CONTROL THE  
 CALCULATION OF THE DIAGONAL ELEMENTS OF THE  
 DECOMPOSITION (AUX[2] > THE MACHINE PRECISION AND  
 AUX[2] > RELATIVE PRECISION OF THE MATRIX ELEMENTS,  
 SEE METHOD AND PERFORMANCE);  
 AUX[3] :  
 EXIT :  
 NORMAL EXIT: ABS(AUX[3]) = N;  
 AUX[3] = N, IF THE MATRIX IS (POSITIVE OR NEGATIVE)  
 DEFINITE;  
 AUX[3] = -N, IF THE INVERSION IS CARRIED OUT, BUT  
 THE MATRIX APPEARS TO BE NON-DEFINITE (SEE METHOD AND  
 PERFORMANCE);  
 FAILURE EXIT : 0 <= AUX[3] < N;  
 IF THE INVERSION CANNOT BE CARRIED OUT BECAUSE SOME  
 DIAGONAL ELEMENTS OF THE DECOMPOSITION ARE TOO SMALL,  
 AUX[3] = K-1, WHERE K IS THE LAST STAGE NUMBER OF THE  
 DECOMPOSITION (SEE METHOD AND PERFORMANCE).

PROCEDURES USED:

SYMDEC1 = CP34701,  
 SYMINV1 = CP34709.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.



## METHOD AND PERFORMANCE:

THE PROCEDURE SYMDECINV1 CALCULATES THE INVERSE OF A SYMMETRIC DEFINITE MATRIX BY CALLING SYMDEC1 AND, IF THIS CALL HAS SUCCESSFUL, SYMINV1.

THE UPPER TRIANGLE OF THE INVERSE MATRIX IS DELIVERED COLUMNWISE IN THE GIVEN ONE-DIMENSIONAL ARRAY.

SEE ALSO METHOD AND PERFORMANCE OF SYMINV2, (THIS SECTION) AND SYMDEC2, SECTION 3.1.1.1.1.3.1.

## EXAMPLE OF USE:

THE UPPER TRIANGLE OF THE SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX (THE PASCAL MATRIX OF ORDER 4) OF THE SYSTEM OF EQUATIONS

$$\begin{array}{rcl}
 x_1 + & x_2 + & x_3 + & x_4 = & 2 \\
 x_1 + 2 * x_2 + & 3 * x_3 + & 4 * x_4 = & 4 \\
 x_1 + 3 * x_2 + & 6 * x_3 + & 10 * x_4 = & 8 \\
 x_1 + 4 * x_2 + & 10 * x_3 + & 20 * x_4 = & 16
 \end{array}$$

IS STORED IN THE ONE-DIMENSIONAL ARRAY PASCAL1.

THE DETERMINANT AND THE INVERSE OF THE COEFFICIENT MATRIX AND THE SOLUTION OF THE LINEAR SYSTEM ARE CALCULATED BY THE FOLLOWING PROGRAM:

```

"BEGIN" "COMMENT" TEST SYMDECSOL1, SYMDETERM1 AND SYMDECINV1;
  "INTEGER" I, J, JJ;
  "ARRAY" PASCAL1[1:(4 + 1) * 4 // 2], B[1:4], AUX[2:3];
  "REAL" DETERMINANT;

  "PROCEDURE" SYMDECSOL1(A, N, AUX, B); "CODE" 34707;
  "REAL" "PROCEDURE" SYMDETERM1(A, N); "CODE" 34703;
  "PROCEDURE" SYMDECINV1(A, N, AUX); "CODE" 34711;

  "PROCEDURE" FILLPASCAL(N); "VALUE" N; "INTEGER" N;
  "BEGIN" "INTEGER" I, J, JJ; JJ := 1;
    "FOR" J := 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" PASCAL1[JJ] := 1;
        "FOR" I := 2 "STEP" 1 "UNTIL" J "DO"
          PASCAL1[JJ + I - 1] := "IF" I = J "THEN"
          PASCAL1[JJ + I - 2] * 2 "ELSE"
          PASCAL1[JJ + I - 2] + PASCAL1[JJ + I - J];
          B[JJ] := 2 ** J;
          JJ := JJ + J
        "END"
      "END" FILL PASCAL;

```

```

AUX[2]:= "-11; FILLPASCAL(4);
SYMDECSOL1(PASCAL1, 4, AUX, B);
"IF" AUX[3] < 4 "THEN"
OUTPUT(61, "("("MATRIX NOT POSITIVE DEFINITE")", /)") "ELSE"
"BEGIN" DETERMINANT:= SYMDETERM1(PASCAL1, 4);
  OUTPUT(61, "("4B")");
  OUTPUT(61, "("("SOLUTION USING SYMDECSOL1:")", /)")";
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  OUTPUT(61, "("4B+D.5D")", B[I]);
  OUTPUT(61, "("//, 4B, "("DETERMINANT USING SYMDETERM1: ")",
    +D.5D, 2/, 4B")", DETERMINANT);

  FILLPASCAL(4);
  SYMDECINV1(PASCAL1, 4, AUX);

  OUTPUT(61, "("("INVERSE MATRIX USING SYMDECINV1:")", //,
    4B")");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" 4 "DO"
    "IF" J < I "THEN" OUTPUT(61, "("12B")") "ELSE"
    OUTPUT(61, "("+ZD.5D3B")", PASCAL1[(J - 1) * J // 2+I]);
    OUTPUT(61, "("//, 4B")")
  "END"
"END"
"END"

```

## THIS PROGRAM DELIVERS:

## SOLUTION USING SYMDECSOL1:

```
+0.00000    +4.00000    -4.00000    +2.00000
```

```
DETERMINANT USING SYMDETERM1: +1.00000
```

## INVERSE MATRIX USING SYMDECINV1:

```
+4.00000    -6.00000    +4.00000    -1.00000
          +14.00000    -11.00000    +3.00000
                          +10.00000    -3.00000
                                  +1.00000
```

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SOURCE TEXT(S) :

```

"CODE" 34708;
"PROCEDURE" SYMINV2(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;
"BEGIN" "INTEGER" I, J, I1;
"ARRAY" U[1 : N];
"PROCEDURE" DUPVECROW(L, U, I, A, B); "CODE" 31031;
"REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
"REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;

I1:= N + 1;
"FOR" I:= N "STEP" = 1 "UNTIL" 1 "DO"
"BEGIN" DUPVECROW(I1, N, I, U, A);
"FOR" J:= N "STEP" = 1 "UNTIL" I1 "DO" A[I, J]:=
= (TAMVEC(I1, J = 1, J, A, U) + MATVEC(J, N, J, A, U));
A[I, I]:= 1 / A[I, I] - MATVEC(I1, N, I, A, U); I1:= I
"END"
"END" SYMINV2;
"EOB"

```

```

"CODE" 34709;
"PROCEDURE" SYMINV1(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;
"BEGIN" "INTEGER" I, II, I1, J, IJ;
"ARRAY" U[1:N];
"REAL" "PROCEDURE" SEQVEC(L, U, I1, SHIFT, A, B); "CODE" 34016;
"REAL" "PROCEDURE" SYMMATVEC(L, U, I, A, B); "CODE" 34018;

I1:= (N + 1) * N // 2; I1:= N + 1;
"FOR" I:= N "STEP" = 1 "UNTIL" 1 "DO"
"BEGIN" IJ:= II + I;
"FOR" J:= I1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" U[IJ]:= A[IJ]; IJ:= IJ + J "END";
"FOR" J:= N "STEP" = 1 "UNTIL" I1 "DO"
"BEGIN" IJ:= IJ - J; A[IJ]:= = SYMMATVEC(I1, N, J, A, U)
"END";
A[II]:= 1 / A[II] - SEQVEC(I1, N, II + I, 0, A, U);
II:= II - I; I1:= I
"END"
"END" SYMINV1;
"EOB"

```

```
"CODE" 34710;  
  "PROCEDURE" SYMDECINV2(A, N, AUX); "VALUE" N; "INTEGER" N;  
  "ARRAY" A, AUX;  
  "BEGIN"  
    "PROCEDURE" SYMDEC2(A, N, AUX); "CODE" 34700;  
    "PROCEDURE" SYMINV2(A, N); "CODE" 34708;  
  
    SYMDEC2(A, N, AUX);  
    "IF" ABS(AUX[3]) = N "THEN" SYMINV2(A, N)  
  "END" SYMDECINV2;  
  "EOP"
```

```
"CODE" 34711;  
  "PROCEDURE" SYMDECINV1(A, N, AUX); "VALUE" N; "INTEGER" N;  
  "ARRAY" A, AUX;  
  "BEGIN"  
    "PROCEDURE" SYMDEC1(A, N, AUX); "CODE" 34701;  
    "PROCEDURE" SYMINV1(A, N); "CODE" 34709;  
  
    SYMDEC1(A, N, AUX);  
    "IF" ABS(AUX[3]) = N "THEN" SYMINV1(A, N)  
  "END" SYMDECINV1;  
  "EOP"
```

SECTION 3.1.1.2.1.1

(MAY 1974)

PAGE 1

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BRIEF DESCRIPTION :

THIS SECTION CONTAINS TWO PROCEDURES :  
 A) LSGORTDEC, FOR THE HOUSEHOLDER TRIANGULARIZATION WITH COLUMN INTERCHANGES OF THE COEFFICIENT MATRIX OF A LINEAR LEAST SQUARES PROBLEM;  
 B) LSGDGLINV, FOR THE CALCULATION OF THE DIAGONAL ELEMENTS OF THE INVERSE OF  $M^{-1}M$ , WHERE M IS THE COEFFICIENT MATRIX OF A LINEAR LEAST SQUARES PROBLEM.

KEY WORDS :

LINEAR LEAST SQUARES PROBLEM,  
 HOUSEHOLDER TRIANGULARIZATION,

SUBSECTION : LSGORTDEC.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS :

"PROCEDURE" LSGORTDEC(A, N, M, AUX, AID, CI); "VALUE" N, M;  
 "INTEGER" N, M; "INTEGER" "ARRAY" CI; "ARRAY" A, AUX, AID;

THE MEANING OF THE FORMAL PARAMETERS IS :

A : <ARRAY IDENTIFIER>;  
 "ARRAY" A[1 : N, 1 : M];  
 ENTRY : THE COEFFICIENT MATRIX OF THE LINEAR LEAST SQUARES PROBLEM;  
 EXIT : IN THE UPPER TRIANGLE OF A (THE ELEMENTS  $A_{II,J}$  WITH  $I < J$ ) THE SUPERDIAGONAL ELEMENTS OF THE UPPER-TRIANGULAR MATRIX, PRODUCED BY THE HOUSEHOLDER TRANSFORMATION; IN THE OTHER PART OF THE COLUMNS OF A THE SIGNIFICANT ELEMENTS OF THE GENERATING VECTORS OF THE HOUSEHOLDER MATRICES USED FOR THE HOUSEHOLDER TRIANGULARIZATION;

N : <ARITHMETIC EXPRESSION>;  
 NUMBER OF ROWS OF THE MATRIX;  
 M : <ARITHMETIC EXPRESSION>;  
 NUMBER OF COLUMNS OF THE MATRIX (N >= M);  
 AUX : <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[2 : 5];  
 ENTRY : AUX[2] CONTAINS A RELATIVE TOLERANCE USED FOR  
 CALCULATING THE DIAGONAL ELEMENTS OF THE  
 UPPER-TRIANGULAR MATRIX;  
 EXIT :  
 AUX[3] DELIVERS THE NUMBER OF THE DIAGONAL ELEMENTS OF  
 THE UPPER-TRIANGULAR MATRIX WHICH ARE FOUND NOT  
 NEGLIGIBLE;  
 NORMAL EXIT AUX[3] = M;  
 AUX[5] := THE MAXIMUM OF THE EUCLIDEAN NORMS OF THE  
 COLUMNS OF THE GIVEN MATRIX;  
 AID : <ARRAY IDENTIFIER>;  
 "ARRAY" AID[1 : M];  
 NORMAL EXIT (AUX[3] = M) : AID CONTAINS THE DIAGONAL  
 ELEMENTS OF THE UPPER-TRIANGULAR MATRIX PRODUCED BY THE  
 HOUSEHOLDER TRIANGULARIZATION;  
 CI : <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" CI[1 : M];  
 EXIT : CI CONTAINS THE PIVOTAL INDICES OF THE  
 INTERCHANGES OF THE COLUMNS OF THE GIVEN MATRIX,

PROCEDURES USED :

TAMMAT = CP34014,  
 ELMCOL = CP34023,  
 ICHCOL = CP34031,

REQUIRED CENTRAL MEMORY :

EXECUTION FIELD LENGTH : AN ARRAY OF M ELEMENTS IS DECLARED,

RUNNING TIME:

(C1 \* M + C2) \* M \* (N = M / 3);  
 THE CONSTANTS C1 AND C2 DEPEND ON THE  
 ARITHMETIC OF THE COMPUTER,

LANGUAGE : ALGOL 60.

## METHOD AND PERFORMANCE :

THE PROCEDURE LSQORTDEC IS A MODIFICATION OF THE PROCEDURE LSQDEC DUE TO T.J. DEKKER (SEE REF [1]), WHERE A DERIVATION IS GIVEN OF A SET OF PROCEDURES BY P. BUSINGER AND G.H. GOLUB (SEE REF [2]), THE METHOD IS HOUSEHOLDER TRIANGULARIZATION WITH COLUMN INTERCHANGES. LET  $M$  DENOTE THE GIVEN MATRIX, LSQORTDEC PRODUCES AN  $N$ -TH ORDER ORTHOGONAL MATRIX  $Q$  AND AN  $N * M$  UPPER-TRIANGULAR MATRIX  $R$  SUCH THAT  $R$  EQUALS  $QM$  WITH PERMUTED COLUMNS,  $Q$  IS THE PRODUCT OF AT MOST  $M$  HOUSEHOLDER MATRICES WHICH ARE REPRESENTED BY THEIR GENERATING VECTORS,  $M$  IS REDUCED TO  $R$  IN AT MOST  $M$  STAGES ; AT THE  $K$ -TH STAGE THE  $K$ -TH COLUMN OF THE (ALREADY MODIFIED) MATRIX IS INTERCHANGED WITH THE COLUMN OF MAXIMUM EUCLIDEAN NORM (THE PIVOTAL COLUMN); THEN THE MATRIX IS MULTIPLIED WITH A HOUSEHOLDER MATRIX SUCH, THAT THE SUBDIAGONAL ELEMENTS OF THE  $K$ -TH COLUMN BECOME ZERO, WHILE THE FIRST  $K - 1$  COLUMNS REMAIN UNCHANGED. THE PROCESS TERMINATES PREMATURELY, IF AT SOME STAGE THE EUCLIDEAN NORM OF THE PIVOTAL COLUMN IS LESS THAN SOME TOLERANCE, VIZ, A GIVEN TOLERANCE (AUX[2]) TIMES THE MAXIMUM OF THE EUCLIDEAN NORMS OF THE COLUMNS OF THE GIVEN MATRIX. LSQORTDEC DELIVERS THE SIGNIFICANT ELEMENTS OF THE GENERATING VECTOR OF THE  $K$ -TH HOUSEHOLDER MATRIX (THE FIRST  $K - 1$  ELEMENTS OF THIS VECTOR BEING ZERO) IN THE LOWER TRIANGLE PART OF THE  $K$ -TH COLUMN OF THE ARRAY  $A$  ( $A[I,K]$  FOR  $I \geq K$ ), OF THE RESULTING UPPER-TRIANGULAR MATRIX THE DIAGONAL ELEMENTS ARE DELIVERED SEPARATELY IN AN ARRAY  $AID$ , AND THE REMAINING ELEMENTS IN THE SUPER-TRIANGULAR PART OF THE ARRAY  $A$ . FOR THE SOLUTION OF LEAST SQUARES PROBLEMS, ONLY CALLS WITH  $N \geq M$  ARE USEFUL.

## REFERENCES :

- [1] DEKKER, T.J. :  
ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 1,  
MC TRACT 22, 1968, MATHEMATISCH CENTRUM, AMSTERDAM.
- [2] BUSINGER, P. AND G.H. GOLUB :  
LINEAR LEAST SQUARES SOLUTION BY HOUSEHOLDER TRANSFORMATIONS,  
NUM. MATH. 7 (1965), PP. 269 - 276.

## EXAMPLE OF USE :

SEE EXAMPLE OF USE OF LSQSOL.

SUBSECTION : LSQDGLINV.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"PROCEDURE" LSQDGLINV(A, M, AID, CI, DIAG); "VALUE" M; "INTEGER" M;  
 "INTEGER" "ARRAY" CI; "ARRAY" A, AID, DIAG;

THE MEANING OF THE FORMAL PARAMETERS IS :

A, M, AID, CI :

SEE CALLING SEQUENCE OF LSQORTDEC (THIS SECTION);  
 THE CONTENTS OF A, AID AND CI SHOULD BE PRODUCED BY A  
 SUCCESSFUL CALL OF LSQORTDEC . (AUX[3] = M) .

DIAG : <ARRAY IDENTIFIER>; "ARRAY" DIAG[1 : M];

EXIT : THE DIAGONAL ELEMENTS OF THE INVERSE OF M'M  
 WHERE M IS THE MATRIX OF THE LINEAR LEAST SQUARES  
 PROBLEM.

PROCEDURES USED :

VECVEC = CP34010,

TAMVEC = CP34012.

RUNNING TIME :

(C3 \* M + C4) \* M \* M;

THE CONSTANTS C3 AND C4 DEPEND ON THE ARITHMETIC  
 OF THE COMPUTER.

LANGUAGE : ALGOL 60.

METHOD AND PERFORMANCE :

LSQDGLINV SHOULD BE CALLED AFTER A SUCCESSFUL CALL OF LSQORTDEC,  
 I.E. IF AUX[3] = M. LSQDGLINV CALCULATES THE DIAGONAL ELEMENTS  
 OF THE INVERSE OF M'M, WHERE M IS THE MATRIX OF A LINEAR  
 LEAST SQUARES PROBLEM.

THESE VALUES CAN BE USED FOR THE COMPUTATION OF THE STANDARD  
 DEVIATIONS OF LEAST SQUARES SOLUTIONS.

EXAMPLE OF USE :

SEE EXAMPLE OF USE OF LSQSOL.



## SOURCE TEXT(S) :

```

"CODE" 34134;
"PROCEDURE" LSQORTDEC(A, N, M, AUX, AID, CI); "VALUE" N, M;
"INTEGER" N, M; "ARRAY" A, AUX, AID; "INTEGER" "ARRAY" CI;
"BEGIN" "INTEGER" J, K, KPIV;
  "REAL" BETA, SIGMA, NORM, W, EPS, AKK, AIDK;
  "ARRAY" SUM[1:M];
  "REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B); "CODE" 34014;
  "PROCEDURE" FLMLCOL(L, U, I, J, A, B, X); "CODE" 34023;
  "PROCEDURE" ICHCOL(L, U, I, J, A); "CODE" 34031;

  NORM:= 0; AUX[3]:= M;
  "FOR" K:= 1 "STEP" 1 "UNTIL" M "DO"
  "BEGIN" W:= SUM[K]:= TAMMAT(1, N, K, K, A, A);
    "IF" W > NORM "THEN" NORM:= W
  "END";
  W:= AUX[5]:= SQRT(NORM); EPS:= AUX[2] * W;
  "FOR" K:= 1 "STEP" 1 "UNTIL" M "DO"
  "BEGIN" SIGMA:= SUM[K]; KPIV:= K;
    "FOR" J:= K + 1 "STEP" 1 "UNTIL" M "DO"
    "IF" SUM[J] > SIGMA "THEN"
    "BEGIN" SIGMA:= SUM[J]; KPIV:= J "END";
    "IF" KPIV = K "THEN"
    "BEGIN" SUM[KPIV]:= SUM[K]; ICHCOL(1, N, K, KPIV, A) "END";
    CI[K]:= KPIV; AKK:= A[K,K];
    SIGMA:= TAMMAT(K, N, K, K, A, A); W:= SQRT(SIGMA);
    AIDK:= AID[K]:= "IF" AKK < 0 "THEN" W "ELSE" = W;
    "IF" W < EPS "THEN"
    "BEGIN" AUX[3]:= K - 1; "GO TO" ENDDC "END";
    BETA:= 1 / (SIGMA - AKK * AIDK); A[K,K]:= AKK - AIDK;
    "FOR" J:= K + 1 "STEP" 1 "UNTIL" M "DO"
    "BEGIN" ELMLCOL(K, N, J, K, A, A, - BETA * TAMMAT(K, N,
      K, J, A, A)); SUM[J]:= SUM[J] - A[K,J] ** 2
    "END"
  "END" FOR K;
ENDDC:
"END" LSQORTDEC;
"EOF"

```

```

"CODE" 34132;
"PROCEDURE" LSQDGLINV(A, M, AID, CI, DIAG); "VALUE" M; "INTEGER" M;
"ARRAY" A, AID, DIAG; "INTEGER" "ARRAY" CI;
"BEGIN" "INTEGER" J, K, CIK;
  "REAL" W;
  "REAL" "PROCEDURE" VECVEC(L, U, S, A, B); "CODE" 34010;
  "REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;

  "FOR" K:= 1 "STEP" 1 "UNTIL" M "DO"
    "BEGIN" DIAG[K]:= 1 / AID[K];
      "FOR" J:= K + 1 "STEP" 1 "UNTIL" M "DO"
        DIAG[J]:= - TAMVEC(K, J - 1, J, A, DIAG) / AID[J];
        DIAG[K]:= VECVEC(K, M, 0, DIAG, DIAG)
      "END";
    "FOR" K:= M "STEP" - 1 "UNTIL" 1 "DO"
      "BEGIN" CIK:= CI[K]; "IF" CIK /= K "THEN"
        "BEGIN" W:= DIAG[K]; DIAG[K]:= DIAG[CIK]; DIAG[CIK]:= W
        "END"
      "END"
    "END" LSQDGLINV;
  "EOP"

```

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BRIEF DESCRIPTION :

THIS SECTION CONTAINS TWO PROCEDURES :  
 A) LSQSOL, FOR THE SOLUTION OF A LINEAR LEAST SQUARES PROBLEM IF THE COEFFICIENT MATRIX HAS BEEN DECOMPOSED BY LSGORTDEC (SECTION 3.1.1.2.1.1.);  
 B) LSGORTDECSOL, FOR THE SOLUTION OF A LINEAR LEAST SQUARES PROBLEM BY HOUSEHOLDER TRIANGULARIZATION WITH COLUMN INTERCHANGES AND FOR THE CALCULATION OF THE DIAGONAL OF THE INVERSE OF  $M^{-1}M$ , WHERE M IS THE COEFFICIENT MATRIX.

KEY WORDS :

LINEAR LEAST SQUARES PROBLEM,  
 HOUSEHOLDER TRIANGULARIZATION.

SUBSECTION : LSQSOL.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS :

"PROCEDURE" LSQSOL(A, N, M, AID, CI, B); "VALUE" N, M;  
 "INTEGER" N, M; "INTEGER" "ARRAY" CI; "ARRAY" A, AID, B;

THE MEANING OF THE FORMAL PARAMETERS IS :

A, N, M, AID, CI : SEE CALLING SEQUENCE OF LSGORTDEC (SECTION 3.1.1.2.1.1.); THE CONTENTS OF THE ARRAYS A, AID AND CI SHOULD BE PRODUCED BY A SUCCESSFUL CALL OF LSGORTDEC, I.E. IF AUX[3] = 4;  
 B : <ARRAY IDENTIFIER>;  
 "ARRAY" B[1 : N];  
 ENTRY : B CONTAINS THE RIGHT HAND SIDE OF A LINEAR LEAST SQUARES PROBLEM;  
 EXIT : B[1 : M] CONTAINS THE SOLUTION OF THE PROBLEM;  
 B[M + 1 : N] CONTAINS A VECTOR WITH EUCLIDEAN LENGTH EQUAL TO THE EUCLIDEAN LENGTH OF THE RESIDUE VECTOR.

PROCEDURES USED :

MATVEC = CP34011,  
 TAMVEC = CP34012,  
 ELMVECCOL = CP34021.

RUNNING TIME :

(C5 \* M + C6) \* N;  
 THE CONSTANTS C5 AND C6 DEPEND UPON THE ELEMENTARY  
 ARITHMETIC OF THE COMPUTER.

LANGUAGE : ALGOL 60.

METHOD AND PERFORMANCE :

LSQSOL SHOULD BE CALLED AFTER A SUCCESSFUL CALL OF LSQORTDEC  
 (SECTION 3,1.1,2,1.1.), I.E. IF AUX[3] = M, LSQSOL YIELDS  
 THE LEAST SQUARES SOLUTION OF THE OVERDETERMINED SYSTEM WITH THE  
 DECOMPOSED COEFFICIENT MATRIX IN ARRAY A AND THE RIGHT HAND SIDE IN  
 ARRAY B.  
 FIRST THE ORTHOGONAL TRANSFORMATION WITH THE HOUSEHOLDER MATRICES  
 IS PERFORMED ON THE RIGHT HAND SIDE, NEXT THE SYSTEM OF THE FIRST M  
 EQUATIONS AND WITH AN UPPER-TRIANGULAR COEFFICIENT MATRIX IS SOLVED  
 BY BACK SUBSTITUTION, YIELDING A SOLUTION WITH M PERMUTED  
 COMPONENTS DUE TO THE COLUMN INTERCHANGES OF THE TRIANGULARIZATION.  
 FINALLY THE ORDER OF THE M COMPONENTS IS RESTORED, SEE ALSO METHOD  
 AND PERFORMANCE OF LSQORTDEC (SECTION 3,1.1,2,1.1.).  
 THE LEAST SQUARES SOLUTIONS OF SEVERAL OVERDETERMINED SYSTEMS WITH  
 THE SAME COEFFICIENT MATRIX CAN BE SOLVED BY SUCCESSIVE CALLS OF  
 LSQSOL WITH DIFFERENT RIGHT HAND SIDES.

EXAMPLE OF USE :

THE NEXT PROGRAM SOLVES THE SYSTEM

$$\begin{array}{rcll}
 - 2 * X1 & + & X2 & = & 0 \\
 - & X1 & + & X2 & = & 1 \\
 & X1 & + & X2 & = & 2 \\
 2 * X1 & + & X2 & = & 2 \\
 & X1 & + & 2 * X2 & = & 3
 \end{array}$$

```

"BEGIN" "COMMENT" 730912, TEST LSQORTDEC, LSQSOL, LSQDGLINV;
"ARRAY" A, C[1 : 5, 1 : 2], B, X[1 : 5], DIAG, AID[1 : 2],
AUX[2 : 5];
"INTEGER" "ARRAY" PIV[1 : 2];
"INTEGER" I, J;
"REAL" H;

"REAL" "PROCEDURE" VECVEC(L, U, S, A, B); "CODE" 34010;
"PROCEDURE" LSQORTDEC(A, N, M, AUX, AID, CI); "CODE" 34134;
"PROCEDURE" LSQSOL(A, N, M, AID, CI, B); "CODE" 34131;
"PROCEDURE" LSQDGLINV(A, M, AID, CI, DIAG); "CODE" 34132;

"REAL" "PROCEDURE" SUM(I, A, B, X); "VALUE" A, B;
"INTEGER" I, A, B; "REAL" X;
"BEGIN" "REAL" S; S := 0; "FOR" I := A "STEP" 1 "UNTIL" B "DO"
  S := S + X; SUM := S
"END" SUM;

AUX[2] := "-12; I := J := 1;
"FOR" H := -2, -1, 1, 2, 1, 1, 1, 1, 2 "DO"
"BEGIN" A[I, J] := C[I, J] := H; "IF" I < 5 "THEN" I := I + 1 "ELSE"
  "BEGIN" I := 1; J := J + 1 "END"
"END";
"FOR" H := 0, 1, 2, 2, 3 "DO"
"BEGIN" B[I] := X[I] := H; I := I + 1 "END";

LSQORTDEC(A, 5, 2, AUX, AID, PIV);
"IF" AUX[3] = 2 "THEN"
"BEGIN" LSQSOL(A, 5, 2, AID, PIV, X);
  LSQDGLINV(A, 2, AID, PIV, DIAG);
  OUTPUT(61, "(" /, "(" AUX[2, 3, 5] = ")" + .4D" + DD5B, 3ZD5B,
    +.4D" + DD /, "(" LSQ SOLUTION :)"", 2(28+.8D" + DD), /
    "(" RESIDUE (DELIVERED) :)"", +.8D" + DD /,
    "(" RESIDUE (CHECKED) :)"", +.8D" + DD /,
    "(" DIAGONAL OF INVERSE MIM :)"", 2(2B+.8D" + DD)"))",
    AUX[2], AUX[3], AUX[5], X[1], X[2],
    SQR(VECVEC(3, 5, 0, X, X)),
    SQR(SUM(I, 1, 5, (B[I] - C[I, 1] * X[1] - C[1, 2] * X[2])
    ** 2)), DIAG[1], DIAG[2])
"END"
"END"
"EQP" END OF PROGRAM

```

DELIVERS :

```

AUX[2, 3, 5] = +.1000"-11      2      +.3317"+01
LSQ SOLUTION : +.50000000"+00 +.12500000"+01
RESIDUE (DELIVERED) :+.50000000"+00
RESIDUE (CHECKED) :+.50000000"+00
DIAGONAL OF INVERSE MIM : +.95238095"-01 +.13095238"+00

```

SUBSECTION : LSQORTDECSOL,

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

```
"PROCEDURE" LSQORTDECSOL(A, N, M, AUX, DIAG, B); "VALUE" N, M;
"INTEGER" N, M; "ARRAY" A, AUX, DIAG, B;
```

THE MEANING OF THE FORMAL PARAMETERS IS :

```
A : <ARRAY IDENTIFIER>;
    "ARRAY" A[1 : N, 1 : M];
    ENTRY : A CONTAINS THE COEFFICIENT MATRIX OF THE
    LINEAR LEAST SQUARES PROBLEM;
    EXIT : IN THE UPPER TRIANGLE OF A (THE ELEMENTS
    A[I, J] WITH I < J) THE SUPERDIAGONAL
    ELEMENTS OF THE UPPER-TRIANGULAR MATRIX, PRODUCED BY
    THE HOUSEHOLDER TRANSFORMATION; IN THE OTHER PART OF
    THE COLUMNS OF A THE SIGNIFICANT ELEMENTS OF THE
    GENERATING VECTORS OF THE HOUSEHOLDER MATRICES USED
    FOR THE HOUSEHOLDER TRIANGULARIZATION;

N : <ARITHMETIC EXPRESSION>;
    NUMBER OF ROWS OF THE MATRIX;

M : <ARITHMETIC EXPRESSION>;
    NUMBER OF COLUMNS OF THE MATRIX (N >= M);

AUX : <ARRAY IDENTIFIER>;
      "ARRAY" AUX[2 : 5];
      ENTRY : AUX[2] CONTAINS A RELATIVE TOLERANCE USED FOR
      CALCULATING THE DIAGONAL ELEMENTS OF THE
      UPPER-TRIANGULAR MATRIX;
      EXIT :
      AUX[3] DELIVERS THE NUMBER OF THE DIAGONAL ELEMENTS OF
      THE UPPER-TRIANGULAR MATRIX WHICH ARE FOUND NOT
      NEGLIGIBLE; NORMAL EXIT AUX[3] = M;
      AUX[5] := THE MAXIMUM OF THE EUCLIDEAN NORMS OF THE
      COLUMNS OF THE GIVEN MATRIX;

DIAG : <ARRAY IDENTIFIER>;
       "ARRAY" DIAG[1 : M];
       EXIT : THE DIAGONAL ELEMENTS OF THE INVERSE OF M*M
       WHERE M IS THE MATRIX OF THE LINEAR LEAST SQUARES
       PROBLEM;

B : <ARRAY IDENTIFIER>;
    "ARRAY" B[1 : N];
    ENTRY : B CONTAINS THE RIGHT HAND SIDE OF A LINEAR
    LEAST SQUARES PROBLEM;
    EXIT : B[1 : M] CONTAINS THE SOLUTION OF THE PROBLEM;
    B[M + 1 : N] CONTAINS A VECTOR WITH EUCLIDEAN LENGTH
    EQUAL TO THE EUCLIDEAN LENGTH OF THE RESIDUE VECTOR.
```

PROCEDURES USED :

```
LSQORTDEC = CP34134,
LSQDGLINV = CP34132,
LSQSOL    = CP34131.
```

REQUIRED CENTRAL MEMORY :

EXECUTION FIELD LENGTH ; AN INTEGER ARRAY AND A REAL ARRAY, BOTH OF M ELEMENTS, ARE DECLARED.

RUNNING TIME : ROUGHLY PROPORTIONAL TO  $N * M ** 2$ .

LANGUAGE : ALGOL 60.

METHOD AND PERFORMANCE :

LSQORTDECSOL SOLVES AN OVERDETERMINED SYSTEM OF N LINEAR EQUATIONS IN M UNKNOWNNS BY CALLING LSQORTDEC AND, IF THIS CALL WAS SUCCESSFUL LSQDGLINV AND LSQSOL. LSQORTDECSOL DELIVERS THE LEAST SQUARES SOLUTION AND THE DIAGONAL OF THE INVERSE OF M<sup>-1</sup>M, WHERE M IS THE COEFFICIENT MATRIX OF THE SYSTEM. SEE SECTION 3.1.1.2.1.1. AND LSQSOL (THIS SECTION).

EXAMPLE OF USE :

THE PROGRAM

```

"BEGIN" "COMMENT" 730914, TEST LSQORTDECSOL;
  "ARRAY" A, C[1 : 5, 1 : 2], B, X[1 : 5], DIAG[1 : 2],
  AUX[2 : 5];
  "INTEGER" I, J;
  "REAL" H;
  "REAL" "PROCEDURE" VECVEC(L, U, S, A, B); "CODE" 34010;
  "PROCEDURE" LSQORTDECSOL(A, N, M, AUX, DIAG, B); "CODE" 34135;
  "REAL" "PROCEDURE" SUM(I, A, B, X); "VALUE" A, B;
  "INTEGER" I, A, B; "REAL" X;
  "BEGIN" "REAL" S; S := 0; "FOR" I := A "STEP" 1 "UNTIL" B "DO"
    S := S + X; SUM := S
  "END" SUM;
  AUX[2] := "-12; I := J := 1;
  "FOR" H := - 2, - 1, 1, 2, 1, 1, 1, 1, 1, 2 "DO"
  "BEGIN" A[I, J] := C[I, J] := H; "IF" I < 5 "THEN" I := I + 1 "ELSE"
    "BEGIN" I := 1; J := J + 1 "END"
  "END";
  "FOR" H := 0, 1, 2, 2, 3 "DO"
  "BEGIN" B[I] := X[I] := H; I := I + 1 "END";
  LSQORTDECSOL(A, 5, 2, AUX, DIAG, X);
  "IF" AUX[3] = 2 "THEN"
  OUTPUT(61, "(", "(", "AUX[2, 3, 5] = ")", +.4D"+DD5B, 3ZD5B,
    +.4D"+DD/, "(", "LSQ SOLUTION :", 2(2B+.8D"+DD), /
    "(", "RESIDUE (DELIVERED) :", +.8D"+DD/,
    "(", "RESIDUE (CHECKED) :", +.8D"+DD/,
    "(", "DIAGONAL OF INVERSE M-1M :", 2(2B+.8D"+DD)"),",
    AUX[2], AUX[3], AUX[5], X[1], X[2],
    SQRT(VECVEC(3, 5, 0, X, X)),
    SQRT(SUM(I, 1, 5, (B[I] - C[I, 1] * X[1] - C[I, 2] * X[2])
    ** 2)), DIAG[1], DIAG[2])
  "END"
  "EQP" END OF PROGRAM

```

WHICH SOLVES THE PROBLEM OF THE EXAMPLE OF USE OF LSQSOL,  
DELIVERS :

```
AUX[2, 3, 5] = +.1000"-11      2      +.3317"+01
LSQ SOLUTION  : +.50000000"+00  +.12500000"+01
RESIDUE (DELIVERED) :+.50000000"+00
RESIDUE (CHECKED)   :+.50000000"+00
DIAGONAL OF INVERSE M'M : +.95238095"-01  +.13095238"+00
```

SOURCE TEXT(S) :

```
"CODE" 34131;
"PROCEDURE" LSQSOL(A, N, M, AID, CI, B); "VALUE" N, M;
"INTEGER" N, M; "ARRAY" A, AID, B; "INTEGER" "ARRAY" CI;
"BEGIN" "INTEGER" K, CIK;
    "REAL" W;
    "REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
    "REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;
    "PROCEDURE" ELMVECCOL(L, U, I, A, B, X); "CODE" 34021;

    "FOR" K:= 1 "STEP" 1 "UNTIL" M "DO" ELMVECCOL(K, N, K, B, A,
    TAMVEC(K, N, K, A, B) / (AID[K] * A[K,K]));
    "FOR" K:= M "STEP" - 1 "UNTIL" 1 "DO" B[K]:= (B[K] - MATVEC
    (K + 1, M, K, A, B)) / AID[K];
    "FOR" K:= M "STEP" - 1 "UNTIL" 1 "DO"
    "BEGIN" CIK:= CI[K]; "IF" CIK ^= K "THEN"
        "BEGIN" W:= B[K]; B[K]:= B[CIK]; B[CIK]:= W "END"
    "END"
"END" LSQSOL;
"EOP"

"CODE" 34135;
"PROCEDURE" LSQORTDECSOL(A, N, M, AUX, DIAG, B); "VALUE" N, M;
"INTEGER" N, M; "ARRAY" A, AUX, DIAG, B;
"BEGIN" "ARRAY" AID[1:M];
    "INTEGER" "ARRAY" CI[1:M];
    "PROCEDURE" LSQORTDEC(A, N, M, AUX, AID, CI); "CODE" 34134;
    "PROCEDURE" LSQDGLINV(A, M, AID, CI, DIAG); "CODE" 34132;
    "PROCEDURE" LSQSOL(A, N, M, AID, CI, B); "CODE" 34131;

    LSQORTDEC(A, N, M, AUX, AID, CI);
    "IF" AUX[3] = M "THEN"
    "BEGIN" LSQDGLINV(A, M, AID, CI, DIAG);
        LSQSOL(A, N, M, AID, CI, B)
    "END"
"END" LSQORTDECSOL;
"EOP"
```



SECTION : 3.1.1.2.1.3

(OCTOBER 1974)

PAGE 1

CONTRIBUTOR : J. KOK.

INSTITUTE : MATHEMATICAL CENTRE.

RECEIVED : 740617.

BRIEF DESCRIPTION :

THIS SECTION CONTAINS ONE PROCEDURE, LSGINV, FOR THE CALCULATION OF THE INVERSE OF THE MATRIX S'S, WHERE S IS THE COEFFICIENT MATRIX OF A LINEAR LEAST SQUARES PROBLEM.

KEYWORDS :

INVERSE MATRIX,  
LEAST SQUARES PROBLEM.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE READS :  
"PROCEDURE" LSGINV(A, M, AID, C); "VALUE" M; "INTEGER" M;  
"ARRAY" A, AID; "INTEGER""ARRAY" C;

THE MEANING OF THE FORMAL PARAMETERS IS :

A : <ARRAY IDENTIFIER>;  
"ARRAY" A[1 : M, 1 : M];  
ENTRY : IN THE UPPER TRIANGLE OF A (THE ELEMENTS A[I,J] WITH  $1 \leq I < J \leq M$ ) THE SUPERDIAGONAL ELEMENTS SHOULD BE GIVEN OF THE UPPERTRIANGULAR MATRIX THAT IS PRODUCED BY THE HOUSEHOLDER TRIANGULARIZATION IN A CALL OF THE PROCEDURE LSGORTDEC (SECTION 3.1.1.2.1.1.) WITH A NORMAL EXIT (AUX[3] = M). SEE ALSO THE MEANING OF THE PARAMETER AID;  
EXIT : THE UPPER TRIANGLE OF THE (SYMMETRIC) INVERSE MATRIX IS DELIVERED IN THE UPPERTRIANGULAR ELEMENTS OF THE ARRAY A (A[I,J] FOR  $1 \leq I \leq J \leq M$ );

M : <ARITHMETIC EXPRESSION>;  
NUMBER OF COLUMNS OF THE MATRIX OF THE LINEAR LEAST SQUARES PROBLEM;

AID : <ARRAY IDENTIFIER>;  
"ARRAY" AID[1 : M];  
ENTRY : AID CONTAINS THE DIAGONAL ELEMENTS OF THE UPPERTRIANGULAR MATRIX THAT IS PRODUCED BY LSGORTDEC;

C : <ARRAY IDENTIFIER>;  
"INTEGER""ARRAY" C[1 : M];  
ENTRY : C CONTAINS THE PIVOTAL INDICES AS PRODUCED BY A CALL OF LSGORTDEC.

SECTION : 3.1.1.2.1.3

(OCTOBER 1974)

PAGE 2

PROCEDURES USED :

CHLINV2 = CP34400,  
 ICHCOL = CP34031,  
 ICHROW = CP34032,  
 ICHROWCOL = CP34033.

REQUIRED CENTRAL MEMORY :

EXECUTION FIELD LENGTH : A REAL ARRAY OF M ELEMENTS IS  
 DECLARED (IN THE CALL OF CHLINV2).

RUNNING TIME : PROPORTIONAL TO M CUBED.

LANGUAGE : ALGOL 60.

METHOD AND PERFORMANCE :

LSGINV SHOULD BE CALLED AFTER A SUCCESSFUL CALL OF LSGORTDEC  
 (SECTION 3.1.1.2.1.1.). LSGINV CAN BE USED FOR THE CALCULATION OF  
 THE COVARIANCE MATRIX OF A LINEAR LEAST SQUARES PROBLEM.  
 LET S BE THE MATRIX OF THE LEAST SQUARES SYSTEM WITH PERMUTED  
 COLUMNS AND  $Q * R$  THE HOUSEHOLDER DECOMPOSITION OF S. THEN THE  
 INVERSE OF  $S'S$  ALSO IS THE INVERSE OF  $R'R$ . SINCE R IS THE  
 CHOLESKY MATRIX OF  $R'R$ , THE INVERSE MATRIX IS COMPUTED IN A CALL  
 OF CHLINV2 (SECTION 3.1.1.1.2.4.). AFTERWARDS THE COVARIANCE  
 MATRIX IS OBTAINED BY INTERCHANGES OF THE COLUMNS AND ROWS OF THE  
 INVERSE MATRIX.

EXAMPLE OF USE :

THE FOLLOWING PROGRAM COMPUTES THE INVERSE T OF  $S'S$ , WHERE S IS  
 THE COEFFICIENT MATRIX OF THE SYSTEM IN THE EXAMPLE OF USE OF  
 LSGORTDEC AND LSGDGLINV (SECTION 3.1.1.2.1.1.). THE DIAGONAL OF S  
 CAN BE COMPARED WITH THE RESULT OF LSGDGLINV. TO CHECK THE ANSWERS  
 $S' * (S * T)$  IS PRINTED.

```

"BEGIN" "COMMENT" JKOK, 740530, EXAMPLE OF USE OF LSGORTDEC AND
LSQINV;

"ARRAY" A, C[1 : 5, 1 : 2], AID[1 : 2], T[1 : 2, 1 : 2],
AUX[2 : 5];
"INTEGER" "ARRAY" PIV[1 : 2];
"INTEGER" I, J; "REAL" H;

"REAL" "PROCEDURE" MATMAT(L, U, I, J, A, B); "CODE" 34013;
"REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B); "CODE" 34014;
"PROCEDURE" LSGORTDEC(A, N, M, AUX, AID, CI); "CODE" 34134;
"PROCEDURE" LSQINV(A, M, AID, CI); "CODE" 34136;

AUX[2] := "-12; I := J := 1;
"FOR" H := -2, -1, 1, 2, 1, 1, 1, 1, 1, 2 "DO"
"BEGIN" A[I, J] := C[I, J] := H; "IF" I < 5 "THEN" I := I + 1 "ELSE"
"BEGIN" I := 1; J := J + 1 "END"
"END";

LSGORTDEC(A, 5, 2, AUX, AID, PIV); "IF" AUX[3] = 2 "THEN"
"BEGIN" LSQINV(A, 2, AID, PIV);
T[1, 1] := A[1, 1]; T[2, 2] := A[2, 2]; T[2, 1] := T[1, 2] := A[1, 2];
"FOR" J := 1, 2 "DO" "FOR" I := 1 "STEP" 1 "UNTIL" 5 "DO"
A[I, J] := MATMAT(1, 2, I, J, C, T);
OUTPUT(61, "(" / 4B, "(" AUX[2, 3, 5] = ")",
+.4D" + DD5B, 3ZD5B, +.4D" + DD /,
2 (/ 4B, 30S, /, 2 (/ 4B, 2(2B + .8D" + DD)), /) ")",
AUX[2], AUX[3], AUX[5],
"(" INVERSE :)", ((T[I, J], J := 1 : 2), I := 1 : 2),
"(" CHECK : S' * (S * T) :)",
((TAMMAT(1, 5, I, J, C, A), J := 1 : 2), I := 1 : 2) )
"END"
"END"
"EOP" END OF PROGRAM
    
```

OUTPUT :

AUX[2, 3, 5] = .1000"-11                    2                    +.3317"+01

INVERSE :

+ .95238095"-01    -.23809524"-01  
 -.23809524"-01    +.13095238"+00

CHECK : S' \* (S \* T) :

+ .10000000"+01    +.17763568"-14  
 +.00000000"+00    +.10000000"+01

SOURCE TEXT(S):

```

"CODE" 34136;
"PROCEDURE" LSGINV(A, M, AID, C); "VALUE" M; "INTEGER" M;
"ARRAY" A, AID; "INTEGER" "ARRAY" C;
"BEGIN" "INTEGER" I, CI;
  "REAL" W;

  "PROCEDURE" CHLINV2(A, N); "CODE" 34400;
  "PROCEDURE" ICHCOL(L, U, I, J, A); "CODE" 34031;
  "PROCEDURE" ICHROW(L, U, I, J, A); "CODE" 34032;
  "PROCEDURE" ICHROWCOL(L, U, I, J, A); "CODE" 34033;

  "FOR" I:= 1 "STEP" 1 "UNTIL" M "DO" A[I,I]:= AID[I];
  CHLINV2(A, M);
  "FOR" I:= M "STEP" - 1 "UNTIL" 1 "DO"
  "BEGIN" CI:= C[I]; "IF" CI # I "THEN"
    "BEGIN" ICHCOL(1, I - 1, I, CI, A); ICHROWCOL(I + 1, CI - 1,
      I, CI, A); ICHROW(CI + 1, M, I, CI, A);
      W:= A[I,I]; A[I,I]:= A[CI,CI]; A[CI,CI]:= W
    "END"
  "END"
"END" LSGINV;
"EOP"

```

SECTION 3.1.1.3.1.1

(DECEMBER 1975)

PAGE 1

AUTHOR : D.T.WINTER

INSTITUTE : MATHEMATICAL CENTRE

RECEIVED : 731217

BRIEF DESCRIPTION :

THIS SECTION CONTAINS 2 PROCEDURES FOR THE SOLUTION OF AN OVERDETERMINED SYSTEM OF LINEAR EQUATIONS:  
 SOLOVR CALCULATES THE SINGULAR VALUES DECOMPOSITION AND SOLVES AN OVERDETERMINED SYSTEM OF LINEAR EQUATIONS.  
 SOLSVDOVR SOLVES AN OVERDETERMINED SYSTEM OF LINEAR EQUATIONS, MULTIPLYING THE RIGHT-HAND SIDE BY THE PSEUDO-INVERSE OF THE GIVEN MATRIX; THE SINGULAR VALUES DECOMPOSITION SHOULD BE AVAILABLE.

KEYWORDS :

BEST LEAST-SQUARES SOLUTION  
 SINGULAR VALUES  
 PSEUDO-INVERSE

SUBSECTION : SOLSVDOVR

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :  
 "PROCEDURE" SOLSVDOVR(U, VAL, V, M, N, X, EM);  
 "VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V, X, EM;

THE MEANING OF THE FORMAL PARAMETERS IS :

U: <ARRAY IDENTIFIER>;  
 "ARRAY" U[1:M,1:N];  
 ENTRY: THE MATRIX U IN THE SINGULAR VALUES DECOMPOSITION  $U*S*V'$ .  
 VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:N];  
 ENTRY: THE SINGULAR VALUES.  
 V: <ARRAY IDENTIFIER>;  
 "ARRAY" V[1:N,1:N];  
 ENTRY: THE MATRIX V IN THE SINGULAR VALUES DECOMPOSITION.  
 N: <ARITHMETIC EXPRESSION>;  
 THE NUMBER OF UNKNOWN.  
 M: <ARITHMETIC EXPRESSION>;  
 THE LENGTH OF THE RIGHT-HAND SIDE VECTOR, N SHOULD SATISFY  $N \leq M$ .  
 X: <ARRAY IDENTIFIER>;  
 "ARRAY" X[1:N];  
 ENTRY: THE RIGHT-HAND SIDE VECTOR;  
 EXIT: THE SOLUTION VECTOR.  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[6:6];  
 ENTRY: EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE.

SECTION 3.1.1.3.1.1

(DECEMBER 1975)

PAGE 2

## PROCEDURES USED :

MATVEC = CP34011

TAMVEC = CP34012

RUNNING TIME : ROUGHLY PROPORTIONAL TO  $(M + N) * N$ 

## METHOD AND PERFORMANCE :

THE SOLUTION IS FOUND IN THREE STEPS :

1.  $U' * X = X1$  IS CALCULATED,
2.  $VAL+ * X1 = X2$  IS CALCULATED, HERE VAL+ DENOTES THE DIAGONAL MATRIX OBTAINED FROM VAL BY SETTING  $VAL+[I,I] = 1/VAL[I]$  IF  $VAL[I]$  GREATER THAN OR EQUAL TO  $EM[6]$ , AND 0 OTHERWISE,
3. THE SOLUTION  $V * X2$  IS CALCULATED.

LANGUAGE : ALGOL 60

SUBSECTION : SOLOVR

## CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"INTEGER" "PROCEDURE" SOLOVR(A, M, N, X, EM);

"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, X, EM;

SOLOVR: THE NUMBER OF SINGULAR VALUES NOT FOUND, I.E. ZERO IF ALL SINGULAR VALUES ARE CALCULATED.

THE MEANING OF THE FORMAL PAREMETERS IS :

- A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:M,1:N];  
 ENTRY: THE MATRIX OF THE SYSTEM;
- M: <ARITHMETIC EXPRESSION>;  
 THE NUMBER OF ROWS OF A;
- N: <ARITHMETIC EXPRESSION>;  
 THE NUMBER OF COLUMNS OF A,  $N \leq M$ ;
- X: <ARRAY IDENTIFIER>;  
 "ARRAY" X[1:M];  
 ENTRY: THE RIGHT-HAND SIDE VECTOR;  
 EXIT: THE SOLUTION VECTOR IN X[1:N];
- EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:7];  
 ENTRY: EM[0]: THE MACHINE PRECISION;  
 EM[2]: THE RELATIVE PROCISSION OF THE SINGULAR VALUES;  
 EM[4]: THE MAXIMAL NUMBER OF ITERATIONS TO BE PERFORMED IN THE SINGULAR VALUES DECOMPOSITION;  
 EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE;
- EXIT: EM[1]: THE INFINITY NORM OF THE MATRIX;  
 EM[3]: THE MAXIMAL NEGLECTED SUPERDIAGONAL ELEMENT;  
 EM[5]: THE NUMBER OF ITERATIONS PERFORMED IN THE SINGULAR VALUES DECOMPOSITION;  
 EM[7]: THE NUMERICAL RANK OF THE MATRIX, I.E. THE NUMBER OF SINGULAR VALUES GREATER THAN OR EQUAL TO  $EM[6]$ .

## PROCEDURES USED :

QRISNGVALDEC = CP34273  
SOLSVDOVR = CP34280

## REQUIRED CENTRAL MEMORY :

AUXILIARY ARRAYS ARE DECLARED TO A TOTAL OF  $(N + 1) * N$  REALS

## METHOD AND PERFORMANCE :

THE SOLUTION IS FOUND IN TWO STEPS :

1. THE SINGULAR VALUES DECOMPOSITION IS CALCULATED BY MEANS OF THE PROCEDURE QRISNGVALDEC (SECTION 3.5.2);
2. THE SOLUTION IS CALCULATED BY MEANS OF THE PROCEDURE SOLSVDOVR, (THIS SECTION);

RUNNING TIME : ROUGHLY PROPORTIONAL TO  $(M + N) * N * N$

LANGUAGE : ALGOL 60

## REFERENCES :

WILKINSON, J.H. AND C.REINSCH  
HANDBOOK OF AUTOMATIC COMPUTATION, VOL. 2 (CONTRIBUTION I-10)  
LINEAR ALGEBRA  
HEIDELBERG (1971)

## EXAMPLE OF USE :

FIRST A PROGRAM IS GIVEN, AND THEN THE RESULTS OF THIS PROGRAM :

```

"BEGIN" "ARRAY" A[1:8,1:5], B[1:8], EM[0:7];
  "INTEGER" I;
  "INTEGER" "PROCEDURE" SOLOVR(A, M, N, X, EM);
  "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, X, EM;
  "CODE" 34281;
  A[1,1]:=22; A[1,2]:= A[2,3]:=10; A[1,3]:= A[7,1]:= A[8,5]:=2;
  A[1,4]:= A[3,5]:=3; A[1,5]:= A[2,2]:=7; A[2,1]:=14; A[2,5]:=8;
  A[2,4]:= A[8,3]:=0; A[3,1]:= A[3,3]:= A[6,5]:=-1; A[3,2]:=13;
  A[3,4]:=-11; A[4,1]:=-3; A[4,2]:= A[4,4]:= A[5,4]:= A[8,4]:=-2;
  A[4,3]:=13; A[4,5]:= A[5,5]:= A[8,1]:=4; A[5,1]:= A[6,1]:=9;
  A[5,2]:=8; A[5,3]:= A[6,2]:= A[7,5]:=1; A[6,3]:=-7;
  A[6,4]:= A[7,4]:= A[8,2]:=5; A[7,2]:=-6; A[7,3]:=6;
  B[1]:=-1; B[2]:=2; B[3]:= B[7]:=1; B[4]:=4; B[5]:= B[8]:=0;
  B[6]:=-3; EM[0]:="-14; EM[2]:="-12; EM[4]:=80; EM[6]:="-10;
  I:= SOLOVR(A, 8, 5, B, EM);
  OUTPUT(61, "("4B, "("NUMBER SINGULAR VALUES NOT FOUND : ")",
  3ZD,/, 4B, "("NORM : ")", N,/, 4B, "("MAX NEGL SUBD ELEM : ")",
  N,/, 4B, "("NUMBER ITERATIONS : ")", 3ZD, /, 4B, "("RANK : ")",
  3ZD, /")", I, EM[1], EM[3], EM[5], EM[7]);
  OUTPUT(61, "("/, 4B, "("SOLUTION VECTOR")",/,/, 5(4B, N, /)")",
  B[1], B[2], B[3], B[4], B[5])

```

SECTION 3.1.1.3.1.1

(MAY 1974)

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```

NUMBER SINGULAR VALUES NOT FOUND :    0
NORM : +4.4000000000000000"+001
MAX NEGL SUBD ELEM : +4.3977072741076"-014
NUMBER ITERATIONS :    6
RANK :    3

```

SOLUTION VECTOR

```

-8.33333333333334"-002
+1.0989227456287"-015
+2.5000000000000000"-001
-8.33333333333332"-002
+8.33333333333334"-002

```

SOURCE TEXT(S):

```

"CODE" 34280;
"PROCEDURE" SOLSVDOVR(U, VAL, V, M, N, X, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V, X, EM;
"BEGIN" "INTEGER" I;
  "REAL" MIN;
  "ARRAY" X1[1:N];
  "REAL" "PROCEDURE" MATVEC(L, U, I, A, B);
  "VALUE" L, U, I; "INTEGER" L, U, I; "ARRAY" A, B;
"CODE" 34011;
"REAL" "PROCEDURE" TAMVEC(L, U, I, A, B);
"VALUE" L, U, I; "INTEGER" L, U, I; "ARRAY" A, B;
"CODE" 34012;
MIN:= EM[6];
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
X1[I]:= "IF" VAL[I] <= MIN "THEN" 0 "ELSE" TAMVEC(1, M, I, U, X) /
VAL[I];
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
X[I]:= MATVEC(1, N, I, V, X1)
"END" SOLSVDOVR;
  "EOP"

"CODE" 34281;
"INTEGER" "PROCEDURE" SOLOVR(A, M, N, X, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, X, EM;
"BEGIN" "INTEGER" I;
  "ARRAY" VAL[1:N], V[1:N,1:N];
  "INTEGER" "PROCEDURE" QRISNGVALDEC(A, M, N, VAL, V, EM);
  "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, VAL, V, EM;
"CODE" 34273;
"PROCEDURE" SOLSVDOVR(U, VAL, V, M, N, X, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V, X, EM;
"CODE" 34280;

SOLOVR:= I:= QRISNGVALDEC(A, M, N, VAL, V, EM);
"IF" I = 0 "THEN" SOLSVDOVR(A, VAL, V, M, N, X, EM)
  SOLOVR;
  "EOP"

```



SECTION 3.1.1.3.1.2

(DECEMBER 1975)

PAGE 1

AUTHOR : D.T.WINTER

INSTITUTE : MATHEMATICAL CENTRE

RECEIVED : 731217

BRIEF DESCRIPTION :

THIS SECTION CONTAINS 2 PROCEDURES FOR THE SOLUTION OF AN UNDERDETERMINED SYSTEM OF LINEAR EQUATIONS:  
SOLUND EXPECTS AS INPUT THE MATRIX OF THE SYSTEM OF EQUATIONS, CALCULATES THE SINGULAR VALUES DECOMPOSITION BY MEANS OF THE PROCEDURE QRISNGVALDEC, AND SOLVES THE SYSTEM BY MEANS OF THE PROCEDURE SOLSVDUND.  
SOLSVDUND ASSUMES THAT THE MATRIX IS ALREADY DECOMPOSED AND SOLVES THE SYSTEM OF EQUATIONS, MULTIPLYING THE RIGHT-HAND SIDE BY THE PSEUDO-INVERSE OF THE GIVEN MATRIX.

KEYWORDS :

BEST LEAST-SQUARES SOLUTION  
SINGULAR VALUES  
PSEUDO-INVERSE

## SECTION 3.1.1.3.1.2

(DECEMBER 1975)

PAGE 2

## SUBSECTION : SOLSVDUND

## CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

```
"PROCEDURE" SOLSVDUND(U, VAL, V, M, N, X, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V, X, EM;
```

THE MEANING OF THE FORMAL PARAMETERS IS :

```
U: <ARRAY IDENTIFIER>;
   "ARRAY" U[1:M,1:N];
   ENTRY: THE MATRIX U IN THE SINGULAR VALUES DECOMPOSITION  $V^*S^*U'$ .
VAL: <ARRAY IDENTIFIER>;
     "ARRAY" VAL[1:N];
     ENTRY: THE SINGULAR VALUES;
V: <ARRAY IDENTIFIER>;
   "ARRAY" V[1:N,1:N];
   ENTRY: THE MATRIX V IN THE SINGULAR VALUES DECOMPOSITION.
N: <ARITHMETIC EXPRESSION>;
   THE LENGTH OF THE RIGHT-HAND SIDE VECTOR;
M: <ARITHMETIC EXPRESSION>;
   THE NUMBER OF UNKNOWN, N SHOULD SATISFY  $N \leq M$ ;
X: <ARRAY IDENTIFIER>;
   "ARRAY" X[1:M];
   ENTRY: THE RIGHT-HAND SIDE VECTOR IN X[1:N];
   EXIT: THE SOLUTION VECTOR IN X[1:M];
EM: <ARRAY IDENTIFIER>;
     "ARRAY" EM[6:6];
     ENTRY: EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE.
```

## PROCEDURES USED :

```
MATVEC = CP34011
TAMVEC = CP34012
```

REQUIRED CENTRAL MEMORY : AN AUXILIARY ARRAY OF N REALS IS DECLARED

RUNNING TIME : ROUGHLY PROPORTIONAL TO  $(M + N) * N$

## METHOD AND PERFORMANCE :

THE SOLUTION IS FOUND IN THREE STEPS :

1.  $V^* * X = X1$  IS CALCULATED,
2.  $VAL+ * X1 = X2$  IS CALCULATED, HERE VAL+ DENOTES THE DIAGONAL MATRIX OBTAINED FROM VAL BY SETTING  $VAL+[I,I] = 1/VAL[I]$  IF  $VAL[I]$  GREATER THAN OR EQUAL TO EM[6], AND 0 OTHERWISE,
3. THE SOLUTION  $U * X2$  IS CALCULATED.

LANGUAGE : ALGOL 60

## SUBSECTION : SOLUND

## CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :  
 "INTEGER" "PROCEDURE" SOLUND(A, M, N, X, EM);  
 "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, X, EM;

SOLUND:= THE NUMBER OF SINGULAR VALUES NOT FOUND, I.E. ZERO IF ALL SINGULAR VALUES ARE CALCULATED.

THE MEANING OF THE FORMAL PAREMETERS IS :

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:M,1:N];  
 ENTRY: THE TRANSPOSE OF THE MATRIX;  
 M: <ARITHMETIC EXPRESSION>;  
 THE NUMBER OF ROWS OF A;  
 N: <ARITHMETIC EXPRESSION>;  
 THE NUMBER OF COLUMNS OF A,  $N \leq M$ ;  
 X: <ARRAY IDENTIFIER>;  
 "ARRAY" X[1:M];  
 ENTRY: THE RIGHT-HAND SIDE VECTOR IN X[1:N];  
 EXIT: THE SOLUTION VECTOR.  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:7];  
 ENTRY: EM[0]: THE MACHINE PRECISION;  
 EM[2]: THE RELATIVE PRECISION FOR THE SINGULAR VALUES;  
 EM[4]: THE MAXIMAL NUMBER OF ITERATIONS TO BE PERFORMED IN  
 THE SINGULAR VALUES DECOMPOSITION;  
 EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE;  
 EXIT: EM[1]: THE INFINITY NORM OF THE MATRIX;  
 EM[3]: THE MAXIMAL NEGLECTED SUPERDIAGONAL ELEMENT;  
 EM[5]: THE NUMBER OF ITERATIONS PERFORMED IN THE SINGULAR  
 VALUES DECOMPOSITION;  
 EM[7]: THE NUMERICAL RANK OF THE MATRIX, I.E. THE NUMBER OF  
 SINGULAR VALUES GREATER THAN OR EQUAL TO EM[6].

## PROCEDURES USED :

QRISNGVALDEC = CP34273  
 SOLSVDUND = CP34282

## REQUIRED CENTRAL MEMORY :

AUXILIARY ARRAYS ARE DECLARED TO A TOTAL OF  $(N + 1) * N$  REALS

## METHOD AND PERFORMANCE :

THE SOLUTION IS FOUND IN TWO STEPS :  
 1. THE SINGULAR VALUES DECOMPOSITION IS CALCULATED BY MEANS OF THE  
 PROCEDURE QRISNGVALDEC;  
 2. THE SOLUTION IS CALCULATED BY MEANS OF THE PROCEDURE SOLSVDUND.

SECTION 3.1.1.3.1.2

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RUNNING TIME : ROUGHLY PROPORTIONAL TO  $(M + N) * N * N$ 

LANGUAGE : ALGOL-60

REFERENCES :

WILKINSON, J.H. AND C. REINSCH  
 HANDBOOK OF AUTOMATIC COMPUTATION, VOL. 2  
 LINEAR ALGEBRA  
 HEIDELBERG (1971)

EXAMPLE OF USE :

FIRST WE GIVE A PROGRAM, AND THAN THE RESULTS OF THIS PROGRAM :

```

"BEGIN" "ARRAY" A[1:8,1:5], B[1:8], EM[0:7];
  "INTEGER" I;
  "INTEGER" "PROCEDURE" SOLUND(A, M, N, X, EM);
  "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, X, EM;
  "CODE" 34283;
  A[1,1]:=22; A[1,2]:=A[2,3]:=10; A[1,3]:=A[7,1]:=A[8,5]:=2;
  A[1,4]:=A[3,5]:=3; A[1,5]:=A[2,2]:=7; A[2,1]:=14; A[2,5]:=8;
  A[2,4]:=A[8,3]:=0; A[3,1]:=A[3,3]:=A[6,5]:=-1; A[3,2]:=13;
  A[3,4]:=-11; A[4,1]:=-3; A[4,2]:=A[4,4]:=A[5,4]:=A[8,4]:=-2;
  A[4,3]:=13; A[4,5]:=A[5,5]:=A[8,1]:=4; A[5,1]:=A[6,1]:=9;
  A[5,2]:=8; A[5,3]:=A[6,2]:=A[7,5]:=1; A[6,3]:=-7;
  A[6,4]:=A[7,4]:=A[8,2]:=5; A[7,2]:=-6; A[7,3]:=6;
  B[1]:=-1; B[2]:=2; B[3]:=1; B[4]:=4; B[5]:=0;
  EM[0]:="-14; EM[2]:="-12; EM[4]:=80; EM[6]:="-10;
  I:= SOLUND(A, 8, 5, B, EM);
  OUTPUT(61, "("4B, "("NUMBER SINGULAR VALUES NOT FOUND : ")",
  3ZD, /, 4B, "("NORM : ")", N, /, 4B, "("MAX NEGL SUBD ELEM : ")",
  N, /, 4B, "("NUMBER ITERATIONS : ")", 3ZD, /, 4B, "("RANK : ")",
  3ZD, /)", I, EM[1], EM[3], EM[5], EM[7]);
  OUTPUT(61, ("/, 4B, "("SOLUTION VECTOR)", /, /, 8(4B, N, /)",
  B[1], B[2], B[3], B[4], B[5], B[6], B[7], B[8])
"END"

```

```

NUMBER SINGULAR VALUES NOT FOUND :      0
NORM : +4.4000000000000000"+001
MAX NEGL SUBD ELEM : +4.3977072741076"-014
NUMBER ITERATIONS :      6
RANK :      3

```

SOLUTION VECTOR

```

+1.6410256410255"-002
+1.4807692307694"-002
-4.8397435897438"-002
+1.00000000000002"-002
-6.7948717948740"-003
+1.1602564102565"-002
+2.99999999999996"-002
-8.3974358974328"-003

```

SECTION 3.1.1.3.1.2

(MAY 1974)

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SOURCE TEXT(S):

```
"CODE" 34282;
"PROCEDURE" SOLSDUND(U, VAL, V, M, N, X, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V, X, EM;
"BEGIN" "INTEGER" I;
      "REAL" MIN;
      "ARRAY" X1[1:N];

      "REAL" "PROCEDURE" MATVEC(L, U, I, A, B);
      "VALUE" L, U, I; "INTEGER" L, U, I; "ARRAY" A, B;
      "CODE" 34011;

      "REAL" "PROCEDURE" TAMVEC(L, U, I, A, B);
      "VALUE" L, U, I; "INTEGER" L, U, I; "ARRAY" A, B;
      "CODE" 34012;

      MIN:= EM[6];
      "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
      X1[I]:= "IF" VAL[I] <= MIN "THEN" 0 "ELSE" TAMVEC(1, N, I, V, X) /
      VAL[I];
      "FOR" I:= 1 "STEP" 1 "UNTIL" M "DO"
      X[I]:= MATVEC(1, N, I, U, X1)
"END" SOLSDUND;
      "EOP"
```

```
"CODE" 34283;
"INTEGER" "PROCEDURE" SOLUND(A, M, N, X, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, X, EM;
"BEGIN" "INTEGER" I;
      "ARRAY" VAL[1:N], V[1:N,1:N];

      "INTEGER" "PROCEDURE" QRISNGVALDEC(A, M, N, VAL, V, EM);
      "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, VAL, V, EM;
      "CODE" 34273;
```

```
"PROCEDURE" SOLSDUND(U, VAL, V, M, N, X, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V, X, EM;
"CODE" 34282;
```

```
SOLUND:= I:= QRISNGVALDEC(A, M, N, VAL, V, EM);
"IF" I = 0 "THEN" SOLSDUND(A, VAL, V, M, N, X, EM)
"END" SOLUND;
      "EOP"
```

AUTHOR : D.T.WINTER

INSTITUTE : MATHEMATICAL CENTRE

RECEIVED : 731217

BRIEF DESCRIPTION :

THIS SECTION CONTAINS 2 PROCEDURES FOR THE CALCULATION OF THE HOMOGENEOUS EQUATIONS  $A * X = 0$  AND  $X' * A = 0$ , WHERE A DENOTES A MATRIX, AND X A VECTOR. HOMSOLSVD ASSUMES THAT THE SINGULAR VALUES DECOMPOSITION OF A HAS BEEN GIVEN. HOMSOL FIRST CALCULATES THE SINGULAR VALUES DECOMPOSITION BY MEANS OF THE PROCEDURE QRISNGVALDEC.

KEYWORDS :

HOMOGENEOUS SOLUTION  
SINGULAR VALUES

SUBSECTION : HOMSOLSVD

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :  
"PROCEDURE" HOMSOLSVD(U, VAL, V, M, N);  
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V;

THE MEANING OF THE FORMAL PARAMETERS IS :

U: <ARRAY IDENTIFIER>;  
"ARRAY" U[1:M,1:N];  
ENTRY:THE MATRIX U IN THE SINGULAR VALUES DECOMPOSITION  $U * S * V'$ .  
EXIT: THE COLUMNS OF U THAT CORRESPOND TO THE ELEMENTS OF VAL WITH A VALUE SMALLER THAN SOME SMALL CONSTANT MAY BE SEEN AS THE SOLUTIONS OF  $X' * A = 0$ ;

VAL: <ARRAY IDENTIFIER>;  
"ARRAY" VAL[1:N];  
ENTRY:THE SINGULAR VALUES;  
EXIT:THE ARRAY WILL BE ORDERED IN SUCH A WAY THAT  $VAL[I] < VAL[J]$  IF  $J < I$ ;

V: <ARRAY IDENTIFIER>;  
"ARRAY" V[1:N,1:N];  
ENTRY:THE MATRIX V IN THE SINGULAR VALUES DECOMPOSITION;  
EXIT:THE COLUMNS OF V THAT CORRESPOND TO THE ELEMENTS OF VAL THAT ARE SMALLER THAN SOME SMALL CONSTANT MAY BE SEEN AS THE SOLUTIONS OF THE EQUATION  $A * X = 0$ ;

M: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF ROWS OF U;

N: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF COLUMNS OF U;

SECTION 3.1.1.3.1.3

(DECEMBER 1975)

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PROCEDURES USED :

ICHCOL = CP34031

RUNNING TIME : PROPORTIONAL TO  $N^2$

METHOD AND PERFORMANCE :

THE PROCEDURE DOES NOTHING MORE THAN A SIMPLE SORTING PROCESS ON THE ELEMENTS OF THE ARRAY VAL, AT THE SAME TIME THE COLUMNS OF U AND V ARE INTERCHANGED, ACCORDING TO THE INTERCHANGING OF THE ELEMENTS VAL.

LANGUAGE : ALGOL 60

SUBSECTION : HOMSOL

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :  
"INTEGER" "PROCEDURE" HOMSOL(A, M, N, V, EM);  
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, V, EM;

HOMSOL := THE NUMBER OF SINGULAR VALUES NOT FOUND, I.E. ZERO IF ALL SINGULAR VALUES ARE CALCULATED.

THE MEANING OF THE FORMAL PAREMETERS IS :

A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1:M,1:N];  
ENTRY: THE MATRIX;  
EXIT: THE COLUMNS OF A THAT CORRESPOND TO THE ELEMENTS OF VAL THAT ARE SMALLER THAN SOME SMALL CONSTANT, MAY BE SEEN AS THE SOLUTIONS OF THE EQUATION  $X' * A = 0$ .  
M: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF ROWS OF A.  
N: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF COLUMNS OF A.

**V:** <ARRAY IDENTIFIER>;  
 "ARRAY" V[1:N,1:N];  
**EXIT:** THE COLUMNS OF V THAT CORRESPOND TO ELEMENTS OF VAL  
 SMALLER THAN SOME SMALL CONSTANT MAY BE SEEN AS THE  
 SOLUTIONS OF THE EQUATION  $A * X = 0$ .  
**EM:** <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:7];  
**ENTRY:** EM[0]: THE MACHINE PRECISION;  
 EM[2]: THE RELATIVE PRECISION FOR THE SINGULAR VALUES;  
 EM[4]: THE MAXIMAL NUMBER OF ITERATIONS TO BE PERFORMED IN  
 THE SINGULAR VALUES DECOMPOSITION;  
 EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE;  
**EXIT:** EM[1]: THE INFINITY NORM OF THE MATRIX;  
 EM[3]: THE MAXIMAL NEGLECTED SUPERDIAGONAL ELEMENT;  
 EM[5]: THE NUMBER OF ITERATIONS PERFORMED IN THE SINGULAR  
 VALUES DECOMPOSITION;  
 EM[7]: THE NUMERICAL RANK OF THE MATRIX, I.E. THE NUMBER OF  
 SINGULAR VALUES GREATER THAN OR EQUAL TO EM[6].

## PROCEDURES USED :

QRISNGVALDEC = CP34273  
 HOMSOLSVD = CP34284

## METHOD AND PERFORMANCE :

THE SOLUTION IS FOUND IN TWO STEPS :  
 1. THE SINGULAR VALUES DECOMPOSITION IS CALCULATED BY MEANS OF THE  
 PROCEDURE QRISNGVALDEC;  
 2. THE SINGULAR VALUES ARE ORDERED BY MEANS OF THE PROCEDURE  
 HOMSOLSVD.

RUNNING TIME : ROUGHLY PROPORTIONAL TO  $(M + N) * N * N$

LANGUAGE : ALGOL 60

## REFERENCES :

WILKINSON, J.H. AND C. REINSCH  
 HANDBOOK OF AUTOMATIC COMPUTATION, VOL. 2  
 LINEAR ALGEBRA  
 HEIDELBERG (1971)



## EXAMPLE OF USE :

FIRST WE GIVE A PROGRAM, AND THEN THE RESULTS OF THIS PROGRAM :

```
"BEGIN" "ARRAY" A[1:8,1:5], V[1:5,1:5], EM[0:7];
  "INTEGER" I, J;
  A[1,1]:=22; A[1,2]:=A[2,3]:=10; A[1,3]:=A[7,1]:=A[8,5]:=2;
  A[1,4]:=A[3,5]:=3; A[1,5]:=A[2,2]:=7; A[2,1]:=14; A[2,5]:=8;
  A[2,4]:=A[8,3]:=0; A[3,1]:=A[3,3]:=A[6,5]:=-1; A[3,2]:=13;
  A[3,4]:=-11; A[4,1]:=-3; A[4,2]:=A[4,4]:=A[5,4]:=A[8,4]:=-2;
  A[4,3]:=13; A[4,5]:=A[5,5]:=A[8,1]:=4; A[5,1]:=A[6,1]:=9;
  A[5,2]:=8; A[5,3]:=A[6,2]:=A[7,5]:=1; A[6,3]:=-7;
  A[6,4]:=A[7,4]:=A[8,2]:=5; A[7,2]:=-6; A[7,3]:=6;
  EM[0]:="=14; EM[2]:="=12; EM[4]:=80; EM[6]:="=10;
  I:=HOMSDL(A, 8, 5, V, EM);
  OUTPUT(61, "("4B, "("NUMBER SINGULAR VALUES NOT FOUND : ")",
  3ZD, /, 4B, "("NORM : ")", N, /, 4B, "("MAX NEGL SUBD ELEM : ")",
  N, /, 4B, "("NUMBER ITERATIONS : ")", 3ZD, /, 4B, "("RANK : ")",
  3ZD, /)"", I, EM[1], EM[3], EM[5], EM[7]);
  "FOR" J:=EM[7] + 1 "STEP" 1 "UNTIL" 5 "DO"
  OUTPUT(61, "("/, 4B, "("COLUMN NUMBER : ")", D, 5(/, 4B, 2(N)),
  3(/, 4B, N), /)"", J, A[1,J], V[1,J], A[2,J], V[2,J], A[3,J],
  V[3,J], A[4,J], V[4,J], A[5,J], V[5,J], A[6,J], A[7,J], A[8,J])
"END"
```

```
NUMBER SINGULAR VALUES NOT FOUND : 0
NORM : +4.4000000000000000"+001
MAX NEGL SUBD ELEM : +4.3977072741076"-014
NUMBER ITERATIONS : 6
RANK : 3
```

```
COLUMN NUMBER : 4
+3.47085998000002"-001 +4.1909548511171"-001
-6.0723369623011"-001 +4.4050912303713"-001
+1.2207461910546"-001 -5.2004549247434"-002
+6.1882574433898"-001 +6.7605914021670"-001
-4.6344371870996"-003 +4.1297730284731"-001
+3.3409859838125"-001
-3.3528410857408"-002
-1.3547246422274"-002
```

```
COLUMN NUMBER : 5
-2.5533109413182"-001 +0.0000000000000000"+000
-1.7359809248754"-001 +4.1854806384909"-001
-2.2081225414163"-001 -3.4879005320758"-001
+4.1165471593410"-002 +2.4415303724531"-001
+9.2044247057656"-001 +8.0221712237742"-001
-2.8895953996492"-002
+6.1327596621994"-002
-4.9058079025100"-002
```

## SOURCE TEXT(S):

```

"CODE" 34284;
"PROCEDURE" HOMSOLSVD(U, VAL, V, M, N);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V;
"BEGIN" "INTEGER" I, J;
    "REAL" X;

    "PROCEDURE" ICHCOL(L, U, I, J, A);
    "VALUE" L, U, I, J; "INTEGER" L, U, I, J; "ARRAY" A;
"CODE" 34031;

"FOR" I:= N "STEP" = 1 "UNTIL" 2 "DO"
"FOR" J:= I - 1 "STEP" = 1 "UNTIL" 1 "DO"
"IF" VAL[I] > VAL[J] "THEN"
"BEGIN" X:= VAL[I]; VAL[I]:= VAL[J]; VAL[J]:= X;
    ICHCOL(1, M, I, J, U); ICHCOL(1, N, I, J, V)
"END"
"END" HOMSOLSVD;
    "EOP"

"CODE" 34285;
"INTEGER" "PROCEDURE" HOMSOL(A, M, N, V, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, V, EM;
"BEGIN" "INTEGER" I;
    "ARRAY" VAL[1:N];

    "INTEGER" "PROCEDURE" GRISNGVALDEC(A, M, N, VAL, V, EM);
    "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, VAL, V, EM;
"CODE" 34273;

"PROCEDURE" HOMSOLSVD(U, VAL, V, M, N);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V;
"CODE" 34284;

HOMSOL:= I:= GRISNGVALDEC(A, M, N, VAL, V, EM);
"IF" I = 0 "THEN" HOMSOLSVD(A, VAL, V, M, N)
"END" HOMSOL;
    "EOP"
    
```

AUTHOR : D.T.WINTER

INSTITUTE : MATHEMATICAL CENTRE

RECEIVED : 731217

BRIEF DESCRIPTION :

THIS SECTION CONTAINS TWO PROCEDURES FOR THE CALCULATION OF THE PSEUDO-INVERSE OF A MATRIX: PSDINVSVD ASSUMES THAT THE MATRIX IS GIVEN AS SINGULAR VALUES DECOMPOSITION. PSDINV FIRST CALCULATES THIS DECOMPOSITION.

KEYWORDS :

PSEUDO-INVERSE  
SINGULAR VALUES

SUBSECTION : PSDINVSVD

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :  
"PROCEDURE" PSDINVSVD((U, VAL, V, M, N, EM);  
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V, EM;

THE MEANING OF THE FORMAL PARAMETERS IS :

U: <ARRAY IDENTIFIER>;  
"ARRAY" U[1:M,1:N];  
ENTRY: THE MATRIX U IN THE SINGULAR VALUES DECOMPOSITION  
 $U * S * V^t$ ;  
EXIT: THE TRANSPOSE OF THE PSEUDO-INVERSE.

VAL: <ARRAY IDENTIFIER>;  
"ARRAY" VAL[1:N];  
THE SINGULAR VALUES.

V: <ARRAY IDENTIFIER>;  
"ARRAY" V[1:N,1:N];  
THE MATRIX V IN THE SINGULAR VALUES DECOMPOSITION  $U * S * V^t$ .

M: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF ROWS OF U.

N: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF COLUMNS OF V.

EM: <ARRAY IDENTIFIER>;  
"ARRAY" EM[6:6];  
ENTRY: EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE.

SECTION 3.1.1.3.1.4

(DECEMBER1975)

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PROCEDURES USED :

MATVEC = CP34011

REQUIRED CENTRAL MEMORY : AN AUXILIARY ARRAY OF N REALS IS DECLARED

METHOD AND PERFORMANCE :

THE PSEUDO-INVERSE IS CALCULATED IN TWO STEPS :

1. THE MATRIX  $X = VAL+ * U'$  IS CALCULATED, WHERE  $VAL+$  DENOTES THE DIAGONAL MATRIX OBTAINED FROM  $VAL$  BY PUTTING  $VAL+[I,I] = 1/VAL[I]$  IF  $VAL[I]$  GREATER THAN OR EQUAL TO  $EM[6]$ , AND  $VAL+[I,I] = 0$  OTHERWISE.
2. THE PSEUDO INVERSE ( $V * X$ ) IS CALCULATED.

RUNNING TIME : ROUGHLY PROPORTIONAL TO  $M * N * N$ 

LANGUAGE : ALGOL-60

SUBSECTION : PSDINV

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

```
"INTEGER" "PROCEDURE" PSDINV(A, M, N, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, EM;
```

PSDINV:= THE NUMBER OF SINGULAR VALUES NOT FOUND, I.E. ZERO IF ALL SINGULAR VALUES ARE CALCULATED.

THE MEANING OF THE FORMAL PARAMETERS IS :

```
A <ARRAY IDENTIFIER>;
"ARRAY" A[1:M,1:N];
ENTRY : THE GIVEN MATRIX;
EXIT : THE TRANSPOSE OF THE PSEUDO-INVERSE;
M: <ARITHMETIC EXPRESSION>;
THE NUMBER OF ROWS OF A;
N: <ARITHMETIC EXPRESSION>;
THE NUMBER OF COLUMNS OF A,  $N \leq M$ ;
EM: <ARRAY IDENTIFIER>;
"ARRAY" EM[0:7];
ENTRY: EM[0]: THE MACHINE PRECISION;
EM[2]: THE RELATIVE PRECISION FOR THE SINGULAR VALUES;
EM[4]: THE MAXIMAL NUMBER OF ITERATIONS TO BE PERFORMED;
EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE;
EXIT: EM[1]: THE INFINITY NORM OF THE MATRIX;
EM[3]: THE MAXIMAL NEGLECTED SUPERDIAGONAL ELEMENT;
EM[5]: THE NUMBER OF ITERATIONS PERFORMED IN THE SINGULAR
VALUES DECOMPOSITION;
EM[7]: THE NUMERICAL RANK OF THE MATRIX, I.E. THE NUMBER OF
SINGULAR VALUES GREATER THAN OR EQUAL TO EM[6];
```

SECTION 3.1.1.3.1.4

(MAY 1974)

PAGE 3

PROCEDURES USED :

GRISNGVALDEC = CP34273  
 PSDINVSVD = CP34286

REQUIRED CENTRAL MEMORY :

AUXILIARY ARRAY'S ARE DECLARED TO A TOTAL OF  $(N + 1) * N$  REALS

METHOD AND PERFORMANCE :

FIRST THE SINGULAR VALUES DECOMPOSITION IS CALCULATED, AND THAN THE PSEUDO-INVERSE IS CALCULATED BY PSDINVSVD,

RUNNING TIME : ROUGHLY PROPORTIONAL TO  $(2M + N) * N * N$

LANGUAGE : ALGOL-60

REFERENCES :

WILKINSON, J.H. AND C. REINSCH  
 HANDBOOK OF AUTOMATIC COMPUTATION, VOL.2  
 LINEAR ALGEBRA  
 HEIDELBERG (1971)

EXAMPLE OF USE :

FIRST WE GIVE A PROGRAM, AND THAN THE RESULTS OF THIS PROGRAM :

```

"BEGIN" "ARRAY" A[1:8,1:5], EM[0:7];
  "INTEGER" I, J;

  "INTEGER" "PROCEDURE" PSDINV(A, M, N, EM);
  "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, EM;
  "CODE" 34287;

  A[1,1]:=22; A[1,2]:=A[2,3]:=10; A[1,3]:=A[7,1]:=A[8,5]:=2;
  A[1,4]:=A[3,5]:=3; A[1,5]:=A[2,2]:=7; A[2,1]:=14; A[2,5]:=8;
  A[2,4]:=A[8,3]:=0; A[3,1]:=A[3,3]:=A[6,5]:=-1; A[3,2]:=13;
  A[3,4]:=-11; A[4,1]:=-3; A[4,2]:=A[4,4]:=A[5,4]:=A[8,4]:=-2;
  A[4,3]:=13; A[4,5]:=A[5,5]:=A[8,1]:=4; A[5,1]:=A[6,1]:=9;
  A[5,2]:=8; A[5,3]:=A[6,2]:=A[7,5]:=1; A[6,3]:=-7;
  A[6,4]:=A[7,4]:=A[8,2]:=5; A[7,2]:=6; A[7,3]:=6;
  EM[0]:=-14; EM[2]:=-12; EM[4]:=80; EM[6]:=-10;
  I:=PSDINV(A, 8, 5, EM);
  OUTPUT(61, ("4B, ("NUMBER SINGULAR VALUES NOT FOUND : ")",
  3ZD, /, 4B, ("NORM : ")", N, /, 4B, ("MAX NEGL SUBD ELEM : ")",
  N, /, 4B, ("NUMBER ITERATIONS : ")", 3ZD, /, 4B, ("RANK : ")",
  3ZD, /)"", I, EM[1], EM[3], EM[5], EM[7]);
  OUTPUT(61, (" /, 4B, ("TRANSPOSE OF PSEUDO-INVERSE)", /,
  4B, ("FIRST THREE COLUMNS)", /, /, 8(4B, 3(N), /), /, /,
  4B, ("LAST TWO COLUMNS)", /, /, 8(15B, 2(N), /)"",
  A[1,1], A[1,2], A[1,3], A[2,1], A[2,2], A[2,3], A[3,1], A[3,2],
  A[3,3], A[4,1], A[4,2], A[4,3], A[5,1], A[5,2], A[5,3], A[6,1],
  A[6,2], A[6,3], A[7,1], A[7,2], A[7,3], A[8,1], A[8,2], A[8,3],
  A[1,4], A[1,5], A[2,4], A[2,5], A[3,4], A[3,5], A[4,4], A[4,5],
  A[5,4], A[5,5], A[6,4], A[6,5], A[7,4], A[7,5], A[8,4], A[8,5])
"END"

```

```

NUMBER SINGULAR VALUES NOT FOUND :      0
NORM : +4.400000000000000" +001
MAX NEGL SUBD ELEM : +4.3977072741076" -014
NUMBER ITERATIONS :      6
RANK :      3

```

TRANSPOSE OF PSEUDO-INVERSE  
FIRST THREE COLUMNS

+2.1129807692308" -002	+4.6153846153850" -003	=2.1073717948727" -003
+9.3108974358974" -003	+2.2115384615376" -003	+2.0528846153848" -002
=1.1097756410256" -002	+2.7403846153848" -002	=3.8862179487199" -003
=7.9166666666667" -003	=5.0000000000007" -003	+3.3750000000001" -002
+5.5128205128205" -003	+9.8076923076935" -003	=8.9743589743826" -004
+1.4318910256410" -002	=2.5961538461548" -003	=2.0136217948716" -002
+4.8958333333335" -003	=1.4999999999998" -002	+1.5312499999996" -002
+1.5064102564102" -003	+7.4038461538447" -003	=1.6987179487147" -003

LAST TWO COLUMNS

+7.6041666666662"=003	+3.8060897435894"=003
-2.0833333333295"=004	+1.0016025641026"=002
-2.7604166666667"=002	+4.2067307692303"=003
-5.4166666666662"=003	+1.0416666666667"=002
-5.0000000000005"=003	+3.2051282051275"=003
+1.2812500000000"=002	+6.2099358974354"=003
+1.2395833333332"=002	+2.6041666666656"=003
-4.9999999999993"=003	+1.6025641025649"=003

SOURCE TEXT(S):

```

"CODE" 34286;
"PROCEDURE" PSDINVSVD(U, VAL, V, M, N, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V, EM;
"BEGIN" "INTEGER" I, J;
  "REAL" MIN, VALI;
  "ARRAY" X[1:N];
  "REAL" "PROCEDURE" MATVEC(L, U, I, A, B);
  "VALUE" L, U, I; "INTEGER" L, U, I; "ARRAY" A, B;
"CODE" 34011;
MIN:= EM[6];
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"IF" VAL[I] > MIN "THEN"
"BEGIN" VALI:= 1 / VAL[I];
  "FOR" J:= 1 "STEP" 1 "UNTIL" M "DO" U[J,I]:= U[J,I] * VALI
"END"
"ELSE" "FOR" J:= 1 "STEP" 1 "UNTIL" M "DO" U[J,I]:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" M "DO"
"BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" N "DO" X[J]:= U[I,J];
  "FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
  U[I,J]:= MATVEC(1, N, J, V, X)
"END"
"END" PSDINVSVD;
"EOP"

```

```

"CODE" 34287;
"INTEGER" "PROCEDURE" PSDINV(A, M, N, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, EM;
"BEGIN" "INTEGER" I;
  "ARRAY" VAL[1:N], V[1:N,1:N];
  "INTEGER" "PROCEDURE" QRISNGVALDEC(A, M, N, VAL, V, EM);
  "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, VAL, V, EM;
"CODE" 34273;
"PROCEDURE" PSDINVSVD(U, VAL, V, M, N, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" U, VAL, V, EM;
"CODE" 34286;

```

```

PSDINV:= I:= QRISNGVALDEC(A, M, N, VAL, V, EM);
"IF" I = 0 "THEN" PSDINVSVD(A, VAL, V, M, N, EM)
"END" PSDINV;
"EOP"

```

SECTION 3.1.2.1.1.1.1.1

(DECEMBER 1975)

PAGE 1

AUTHOR : T.J. DEKKER.

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INSTITUTE : MATHEMATICAL CENTRE.

RECEIVED : 730903.

## BRIEF DESCRIPTION :

THIS SECTION CONTAINS THE PROCEDURE DECBND FOR THE DECOMPOSITION OF A BAND MATRIX BY GAUSSIAN ELIMINATION WITH STABILIZING ROW INTERCHANGES (PARTIAL PIVOTING).

## KEY WORDS :

LINEAR EQUATIONS,  
PARTIAL PIVOTING,  
GAUSSIAN ELIMINATION,  
BAND MATRIX.

## CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"PROCEDURE" DECBND(A, N, LW, RW, AUX, M, P); "VALUE" N, LW, RW;  
"INTEGER" N, LW, RW; "INTEGER""ARRAY" P; "ARRAY" A, M, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS :

A : <ARRAY IDENTIFIER>;  
"ARRAY" A[1 : (LW + RW) \* (N - 1) + N];  
ENTRY : A CONTAINS ROWWISE THE BAND ELEMENTS OF THE BAND MATRIX IN SUCH A WAY THAT THE (I,J)-TH ELEMENT OF THE MATRIX IS GIVEN IN A[(LW + RW) \* (I - 1) + J], I=1,...,N AND J=MAX(1,I-LW),...,MIN(N,I+RW). THE VALUES OF THE REMAINING ELEMENTS OF A ARE IRRELEVANT.  
EXIT : THE BAND ELEMENTS OF THE GAUSSIAN ELIMINATED MATRIX, WHICH IS AN UPPERTRIANGULAR BAND MATRIX WITH (LW + RW) CODIAGONALS, ARE ROWWISE DELIVERED IN A AS FOLLOWS: THE (I,J)-TH ELEMENT OF U IS A[(LW + RW) \* (I - J) + J], I=1,...,N AND J=I,...,MIN(N,I + LW + RW).  
N : <ARITHMETIC EXPRESSION>;  
ORDER OF THE BAND MATRIX;  
LW : <ARITHMETIC EXPRESSION>;  
NUMBER OF LEFT CODIAGONALS OF A;



RW : <ARITHMETIC EXPRESSION>;  
 NUMBER OF RIGHT CODIAGONALS OF A;  
 AUX : <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[1 : 5];  
 ENTRY : AUX[2] = EPS IS A RELATIVE TOLERANCE TO CONTROL  
 THE ELIMINATION; THE PROCESS IS DISCONTINUED IF  
 (EPS > PIVOT[I] / EUCLIDEAN NORM OF I-TH ROW)  
 IN THE I-TH ELIMINATION STEP;  
 NORMAL EXIT :  
 AUX[1] = SIGN OF THE DETERMINANT OF THE MATRIX  
 (+1 OR -1);  
 AUX[3] = N;  
 AUX[5] = MINIMUM ABSOLUTE VALUE OF  
 PIVOT[I] / EUCLIDEAN NORM OF THE I-TH ROW;  
 ABNORMAL EXIT : IF THE ELIMINATION CANNOT BE CARRIED  
 OUT, I.E. IF TEMP (THE QUANTITY  
 ABS(PIVOT[I] / EUCLIDEAN NORM OF THE I-TH ROW))  
 IS TOO SMALL IN THE I-TH ELIMINATION STEP :  
 AUX[3] = I - 1,  
 AUX[5] = TEMP;  
 M : <ARRAY IDENTIFIER>;  
 "ARRAY" M[1 : LW \* (N - 2) + 1];  
 EXIT : THE GAUSSIAN MULTIPLIERS OF ALL ELIMINATIONS  
 IN SUCH A WAY THAT THE I-TH MULTIPLIER OF THE J-TH  
 STEP IS M [ LW \* (J - 1) + I - J ].  
 P : <ARRAY IDENTIFIER>;  
 "INTEGER""ARRAY" P[1 : N];  
 EXIT : THE PIVOTAL INDICES.

PROCEDURES USED :

VECVEC = CP34010,  
 ELMVEC = CP34020,  
 ICHVEC = CP34030.

REQUIRED CENTRAL MEMORY :

EXECUTION FIELD LENGTH : A REAL ARRAY OF N ELEMENTS IS DECLARED.

RUNNING TIME :

(C1 \* LW + C2) \* (LW + RW + 1) \* N;  
 THE CONSTANTS C1 AND C2 DEPEND UPON THE  
 ARITHMETIC OF THE COMPUTER.

LANGUAGE : ALGOL 60.

METHOD AND PERFORMANCE :

DECBND PERFORMS THE DECOMPOSITION OF A MATRIX WHOSE NON-ZERO ELEMENTS ARE IN BAND FORM, AND WHOSE BAND ELEMENTS ARE STORED ROWWISE IN A ONE-DIMENSIONAL ARRAY.

THE METHOD USED IS GAUSSIAN ELIMINATION WITH STABILIZING ROW INTERCHANGES (PARTIAL PIVOTING).

THE GAUSSIAN ELIMINATION IS PERFORMED IN N STEPS. IN THE K-TH STEP,  $K = 1, \dots, N$ , A PIVOT IS SELECTED IN THE K-TH COLUMN OF THE REMAINING SUBMATRIX OF ORDER  $N - K + 1$  (THIS COLUMN CONTAINS AT MOST  $LW + 1$  NON-ZERO ELEMENTS); THEN THE PIVOTAL ROW IS INTERCHANGED WITH THE K-TH ROW; SUBSEQUENTLY THE K-TH UNKNOWN IS ELIMINATED IN THE LAST  $N - K$  ROWS (ONLY THE FIRST  $LW$  OF THESE LAST ROWS ARE INVOLVED HERE).

THE PIVOT IS SELECTED IN SUCH A WAY THAT ITS ABSOLUTE VALUE DIVIDED BY THE EUCLIDEAN NORM OF THE CORRESPONDING ROW OF THE MATRIX IS MAXIMAL. THUS, THE MATRIX IS EQUILIBRATED IN THIS PIVOTING STRATEGY SUCH, THAT THE ROWS EFFECTIVELY OBTAIN UNIT EUCLIDEAN NORM.

THE PROCEDURE DELIVERS THE BAND ELEMENTS OF THE ELIMINATED MATRIX (WHICH IS AN UPPER TRIANGULAR MATRIX WITH  $LW + RW$  SUPERDIAGONALS) AND THE GAUSSIAN MULTIPLIERS FOR EACH ELIMINATION

THE ELIMINATION CANNOT BE CARRIED OUT IF THE ABSOLUTE VALUE OF THE PIVOT IS LESS THAN A GIVEN RELATIVE TOLERANCE (AUX[2]) TIMES THE EUCLIDEAN NORM OF THE CORRESPONDING ROW OF THE MATRIX. THEN THE PREVIOUS STEP NUMBER OF THE ELIMINATION IS DELIVERED (IN AUX[3], WHICH ELSE TAKES THE VALUE N). SEE ALSO REF [1], SECTION 212.

REFERENCE :

- [1] DEKKER, T.J. :  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 1,  
 MC TRACT 22, 1968, MATHEMATISCH CENTRUM, AMSTERDAM.

EXAMPLE OF USE :

SEE EXAMPLE OF USE OF SOLBND.

## SOURCE TEXT(S) :

```

"CODE" 34320;
"PROCEDURE" DECBND(A, N, LW, RW, AUX, M, P); "VALUE" N, LW, RW;
"INTEGER" N, LW, RW; "INTEGER" "ARRAY" P; "ARRAY" A, M, AUX;
"BEGIN" "INTEGER" I, J, K, KK, KK1, PK, MK, IK, LW1, F, Q, W, W1,
        W2, NRW, IW, SDET;
        "REAL" R, S, EPS, MIN;
        "ARRAY" V[1:N];

"REAL" "PROCEDURE" VECVEC(A, B, C, D, E); "CODE" 34010;
"PROCEDURE" ELMVEC(A, B, C, D, E, F); "CODE" 34020;
"PROCEDURE" ICHVEC(A, B, C, D); "CODE" 34030;
F:= LW; W1:= LW + RW; W2:= W1 + 1; W3:= W2 + 1; IW:= 0; SDET:= 1;
NRW:= N + RW; LW1:= LW + 1; Q:= LW - 1;
"FOR" I:= 2 "STEP" 1 "UNTIL" LW "DO"
"BEGIN" Q:= Q + 1; IW:= IW + W1;
        "FOR" J:= IW - Q "STEP" 1 "UNTIL" IW "DO" A[J]:= 0
"END";
IW:= - W2; Q:= - LW;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" IW:= IW + W; "IF" I <= LW1 "THEN" IW:= IW - 1;
        Q:= Q + W; "IF" I > NRW "THEN" Q:= Q - 1;
        V[I]:= SQRT(VECVEC(IW, Q, 0, A, A))
"END";
EPS:= AUX[2]; MIN:= 1; KK:= - W1; MK:= - LW;
"IF" F > NRW "THEN" W2:= W2 + NRW - F;
"FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" "IF" F < N "THEN" F:= F + 1; IK:= KK:= KK + W;
        MK:= MK + LW; S:= ABS(A[KK]) / V[K]; PK:= K; KK1:= KK + 1;
        "FOR" I:= K + 1 "STEP" 1 "UNTIL" F "DO"
        "BEGIN" IK:= IK + W1; M[MK + I - K]:= R:= A[IK]; A[IK]:= 0;
                R:= ABS(R) / V[I]; "IF" R > S "THEN"
                "BEGIN" S:= R; PK:= I "END"
        "END";
"IF" S < MIN "THEN" MIN:= S; "IF" S < EPS "THEN"
"BEGIN" AUX[3]:= K - 1; AUX[5]:= S; "GO TO" END "END";
"IF" K + W2 >= N "THEN" W2:= W2 - 1;
P[K]:= PK; "IF" PK = K "THEN"
"BEGIN" V[PK]:= V[K];
        PK:= PK - K; ICHVEC(KK1, KK1 + W2, PK * W1, A);
        SDET:= - SDET; R:= M[MK + PK]; M[MK + PK]:= A[KK];
        A[KK]:= R
"END" "ELSE" R:= A[KK]; "IF" R < 0 "THEN" SDET:= - SDET;
IW:= KK1; LW1:= F - K + MK;
"FOR" I:= MK + 1 "STEP" 1 "UNTIL" LW1 "DO"
"BEGIN" M[I]:= S:= M[I] / R; IW:= IW + W1;
        ELMVEC(IW, IW + W2, KK1 - IW, A, A, - S)
"END"
"END";
AUX[3]:= N; AUX[5]:= MIN;
END; AUX[1]:= SDET
"END" DECBND;
"EOF"
    
```

CONTRIBUTOR : J. KOK.

INSTITUTE : MATHEMATICAL CENTRE.

RECEIVED : 730 903.

BRIEF DESCRIPTION :

THIS SECTION CONTAINS THE PROCEDURE DETERMBND  
FOR THE CALCULATION OF THE DETERMINANT OF A BAND MATRIX.

KEY WORDS :

DETERMINANT,  
BAND MATRIX.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"REAL""PROCEDURE" DETERMBND(A, N, LW, RW, SGNDT); "VALUE" N, LW,  
RW, SGNDT; "INTEGER" N, LW, RW, SGNDT; "ARRAY" A;

DETERMBND DELIVERS THE DETERMINANT OF THE MATRIX.

THE MEANING OF THE FORMAL PARAMETERS IS :

A, N, LW, RW : SEE CALLING SEQUENCE OF DECBND  
(SECTION 3.1.2.1.1.1.1.1.);  
ENTRY : THE CONTENTS OF A ARE AS PRODUCED BY DECBND OR  
DECSOLBND (SECTION 3.1.2.1.1.1.1.3.);  
SGNDT : <ARITHMETIC EXPRESSION>;  
ENTRY : THE SIGN OF THE DETERMINANT AS DELIVERED IN  
AUX[1] BY DECBND, IF THE ELIMINATION BY DECBND WAS  
SUCCESSFUL.

SECTION 3.1.2.1.1.1.1.2

(DECEMBER 1975)

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PROCEDURES USED : NONE.

RUNNING TIME : PROPORTIONAL TO N.

LANGUAGE : ALGOL 60.

METHOD AND PERFORMANCE :

DETERMBND CAN BE CALLED AFTER DECBND OR DECSOLBND ONLY IF THE GAUSSIAN ELIMINATION WAS SUCCESSFUL, I.E. IF AUX[3] = N. THE FUNCTION VALUE OF DETERMBND IS THE DETERMINANT OF THE GAUSSIAN ELIMINATED UPPER TRIANGULAR MATRIX PROVIDED WITH THE CORRECT SIGN THAT IS DELIVERED BY DECBND OR DECSOLBND IN AUX[1]. DETERMBND SHOULD NOT BE CALLED WHEN OVERFLOW CAN BE EXPECTED.

EXAMPLE OF USE :

SEE EXAMPLES OF USE OF SOLBND AND DECSOLBND.

SOURCE TEXT(S) :

```
"CODE" 34321;
"REAL""PROCEDURE" DETERMBND(A, N, LW, RW, SGNDT);
"VALUE" N, LW, RW, SGNDT; "INTEGER" N, LW, RW, SGNDT; "ARRAY" A;
"BEGIN""INTEGER" I, L; "REAL" P;
    L:= 1; P:= 1; LW:= LW + RW + 1;
    "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
        "BEGIN" P:= A[I] * P; L:= L + LW "END";
    DETERMBND:= ABS(P) * SGNDT
"END" DETERMBND;
"EOP"
```

AUTHOR : T.J. DEKKER,  
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 INSTITUTE : MATHEMATICAL CENTRE,  
 RECEIVED : 730903,

BRIEF DESCRIPTION :

THIS SECTION CONTAINS TWO PROCEDURES.  
 A) SOLBND, FOR THE SOLUTION OF ONE OR MORE SYSTEMS OF LINEAR EQUATIONS WITH THE SAME COEFFICIENT MATRIX, IF THIS MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE DECBND (SECTION 3,1,2,1,1,1,1,1.).  
 B) DECSOLBND, FOR THE SOLUTION OF ONE SYSTEM OF LINEAR EQUATIONS BY GAUSSIAN ELIMINATION WITH STABILIZING ROW INTERCHANGES (PARTIAL PIVOTING) IF THE COEFFICIENT MATRIX IS IN BAND FORM AND IS STORED ROWWISE IN A ONE-DIMENSIONAL ARRAY.

KEY WORDS :

LINEAR EQUATIONS,  
 PARTIAL PIVOTING,  
 GAUSSIAN ELIMINATION,  
 BAND MATRIX,

SUBSECTION : SOLBND.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"PROCEDURE" SOLBND(A, N, LW, RW, M, P, B); "VALUE" N, LW, RW;  
 "INTEGER" N, LW, RW; "INTEGER" "ARRAY" P; "ARRAY" A, M, B;

THE MEANING OF THE FORMAL PARAMETERS IS :

A, N, LW, RW, M, P : SEE CALLING SEQUENCE OF DECBND,  
 ENTRY : THE CONTENTS OF THE ARRAYS A, M, P ARE AS PRODUCED BY DECBND;  
 B : <ARRAY IDENTIFIER>;  
 "ARRAY" B[1 : N];  
 ENTRY : THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR EQUATIONS;  
 EXIT : THE SOLUTION OF THE SYSTEM.



SECTION 3.1.2.1.1.1.1.3

(DECEMBER 1975)

PAGE 3

SUBSECTION : DECSOLBND.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"PROCEDURE" DECSOLBND(A, N, LW, RW, AUX, B); "VALUE" N, LW, RW;  
"INTEGER" N, LW, RW; "ARRAY" A, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS :

A, N, LW, RW, AUX : SEE DECBND (SECTION : 3.1.2.1.1.1.1.1);  
B : SEE SOLBND (THIS SECTION).

PROCEDURES USED :

VECVEC = CP34010,  
ELMVEC = CP34020,  
ICHVEC = CP34030.

REQUIRED CENTRAL MEMORY :

EXECUTION FIELD LENGTH : A REAL ARRAY OF N ELEMENTS AND A REAL  
ARRAY OF LW + 1 ELEMENTS ARE DECLARED.

RUNNING TIME :

$(C1 * LW + C6) * (LW + RW + 1) * N$ ;  
THE CONSTANTS C1 AND C6 DEPEND UPON THE  
ARITHMETIC OF THE COMPUTER.

LANGUAGE : ALGOL 60.



## METHOD AND PERFORMANCE :

DECSOLBND PERFORMS GAUSSIAN ELIMINATION IN THE SAME WAY AS DECBND, MEANWHILE ALSO CARRYING OUT THE ELIMINATION WITH THE GIVEN RIGHT HAND SIDE. THE SOLUTION OF THE ELIMINATED SYSTEM IS OBTAINED BY BACK SUBSTITUTION.

## EXAMPLE OF USE :

## THE PROGRAM

```

"BEGIN""COMMENT" 730822, TEST DECSOLBND AND DETERMBND;
  "PROCEDURE" DECSOLBND(A, N, LW, RW, AUX, B); "CODE" 34322;
  "REAL""PROCEDURE" DETERMBND(A, N, LW, RW, SGNDT); "CODE" 34321;
  "INTEGER" I;
  "ARRAY" BAND[1 : 13], RIGHT, AUX[1 : 5];

  "FOR" I:= 1 "STEP" 1 "UNTIL" 13 "DO"
    BAND[I]:= "IF" (I + 1) // 3 * 3 < I "THEN" 2 "ELSE" - 1;
    RIGHT[1]:= RIGHT[5]:= 1;
  "FOR" I:= 2, 3, 4 "DO" RIGHT[I]:= 0; AUX[2]:= "- 12;
  DECSOLBND(BAND, 5, 1, 1, AUX, RIGHT);
  "IF" AUX[3] = 5 "THEN"
    "BEGIN"
      OUTPUT(61, "("5(+2Z.4D2B), /"("DETERMINANT IS ") +.8D"+DD
      ")", (RIGHT[I], I:= 1 : 5), DETERMBND(BAND, 5, 1, 1, AUX[1]))
    "END"
  "END"

```

WHICH SOLVES THE SAME PROBLEM AS THE PROGRAM IN THE EXAMPLE OF USE OF SOLBND, DELIVERS :

```

+1.0000 +1.0000 +1.0000 +1.0000 +1.0000
DETERMINANT IS +.60000000"+01

```

## SOURCE TEXT(S) :

```

"CODE" 34071;
"PROCEDURE" SOLBND(A, N, LW, RW, M, P, B); "VALUE" N, LW, RW;
"INTEGER" N, LW, RW; "INTEGER" "ARRAY" P; "ARRAY" A, B, M;
"BEGIN" "INTEGER" F, I, K, KK, W, W1, W2, SHIFT;
      "REAL" S;

      "REAL" "PROCEDURE" VECVEC(A, B, C, D, E); "CODE" 34010;
      "PROCEDURE" ELMVEC(A, B, C, D, E, F); "CODE" 34020;

      F:= LW; SHIFT:= - LW; W1:= LW - 1;
      "FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" "IF" F < N "THEN" F:= F + 1; SHIFT:= SHIFT + W1;
        I:=P[K]; S:= B[I]; "IF" I # K "THEN"
          "BEGIN" B[I]:= B[K]; B[K]:= S "END";
          ELMVEC(K + 1, F, SHIFT, B, M, = S)
      "END";
      W1:= LW + RW; W:= W1 + 1; KK:= (N + 1) * W - W1; W2:= - 1;
      SHIFT:= N * W1;
      "FOR" K:= N "STEP" - 1 "UNTIL" 1 "DO"
      "BEGIN" KK:= KK - W; SHIFT:= SHIFT - W1;
        "IF" W2 < W1 "THEN" W2:= W2 + 1;
        B[K]:= -(B[K] - VECVEC(K + 1, K + W2, SHIFT, B, A)) / A[KK]
      "END"
"END" SOLBND;
"EQP"

"CODE" 34322;
"PROCEDURE" DECSOLBND(A, N, LW, RW, AUX, B); "VALUE" N, LW, RW;
"INTEGER" N, LW, RW; "ARRAY" A, B, AUX;
"BEGIN" "INTEGER" I, J, K, KK, KK1, PK, IK, LW1, F, Q, W, W1, W2, IW,
      NRW, SHIFT, SDET;
      "REAL" R, S, EPS, MIN; "ARRAY" M[0:LW], V[1:N];

      "REAL" "PROCEDURE" VECVEC(A, B, C, D, E); "CODE" 34010;
      "PROCEDURE" ELMVEC(A, B, C, D, E, F); "CODE" 34020;
      "PROCEDURE" ICHVEC(A, B, C, D); "CODE" 34030;

      F:= LW; SDET:= 1; W1:= LW + RW; W:= W1 + 1; W2:= W - 2; IW:= 0;
      NRW:= N - RW; LW1:= LW + 1; Q:= LW - 1;
      "FOR" I:= 2 "STEP" 1 "UNTIL" LW "DO"
      "BEGIN" Q:= Q - 1; IW:= IW + W1;
        "FOR" J:= IW - Q "STEP" 1 "UNTIL" IW "DO" A[J]:= 0
      "END";

```

"COMMENT"

```

IW:= - W2; Q:= - LW;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" IW:= IW + W; "IF" I <= LW1 "THEN" IW:= IW - 1;
      Q:= Q + W; "IF" I > NRW "THEN" Q:= Q - 1;
      V[I]:= SQRT(VECVEC(IW, Q, 0, A, A))
"END";
EPS:= AUX[2]; MIN:= 1; KK:= - W1;
"IF" F > NRW "THEN" W2:= W2 + NRW - F;
"FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" "IF" F < N "THEN" F:= F + 1; IK:= KK:= KK + W;
      S:= ABS(A[KK]) / V[K]; PK:= K; KK1:= KK + 1;
      "FOR" I:= K + 1 "STEP" 1 "UNTIL" F "DO"
      "BEGIN" IK:= IK + W1; M[I - K]:= R:= A[IK]; A[IK]:= 0;
            R:= ABS(R) / V[I]; "IF" R > S "THEN"
            "BEGIN" S:= R; PK:= I "END"
      "END";
      "IF" S < MIN "THEN" MIN:= S; "IF" S < EPS "THEN"
      "BEGIN" AUX[3]:= K - 1; AUX[5]:= S; "GO TO" END "END";
      "IF" K + W2 >= N "THEN" W2:= W2 - 1; "IF" PK = K "THEN"
      "BEGIN" V[PK]:= V[K];
            PK:= PK - K; ICHVEC(KK1, KK1 + W2, PK * W1, A);
            SDET:= - SDET; R:= B[K]; B[K]:= B[PK + K];
            B[PK + K]:= R; R:= M[PK]; M[PK]:= A[KK]; A[KK]:= R
      "END"
      "ELSE" R:= A[KK]; IW:= KK1; LW1:= F - K;
      "IF" R < 0 "THEN" SDET:= - SDET;
      "FOR" I:= 1 "STEP" 1 "UNTIL" LW1 "DO"
      "BEGIN" M[I]:= S:= M[I] / R; IW:= IW + W1;
            ELMVEC(IW, IW + W2, KK1 - IW, A, A, = S);
            B[K + I]:= B[K + I] - B[K] * S
      "END"
"END";
AUX[3]:= N; AUX[5]:= MIN;
KK:= (N + 1) * W - W1; W2:= - 1; SHIFT:= N * W1;
"FOR" K:= N "STEP" - 1 "UNTIL" 1 "DO"
"BEGIN" KK:= KK - W; SHIFT:= SHIFT - W1;
      "IF" W2 < W1 "THEN" W2:= W2 + 1;
      B[K]:= (B[K] - VECVEC(K + 1, K + W2, SHIFT, B, A)) / A[KK]
"END";
END; AUX[1]:= SDET
"END" DECSOLBND;
"EOF"
    
```

SECTION 3.1.2.1.1.1.2.1

(JUNE 1974)

PAGE 1

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RECEIVED: 731210.

## BRIEF DESCRIPTION:

THIS SECTION CONTAINS TWO PREPARATORY PROCEDURES FOR THE SOLUTION OF SYSTEMS OF LINEAR ALGEBRAIC EQUATIONS WITH A TRIDIAGONAL MATRIX;  
DECTRI PERFORMS A TRIANGULAR DECOMPOSITION OF A TRIDIAGONAL MATRIX.  
DECTRIPIV PERFORMS A TRIANGULAR DECOMPOSITION OF A TRIDIAGONAL MATRIX, USING PARTIAL PIVOTING TO STABILIZE THE PROCESS.

## KEYWORDS:

LU DECOMPOSITION,  
TRIANGULAR DECOMPOSITION,  
TRIDIAGONAL MATRIX.

SUBSECTION: DECTRI.

## CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
"PROCEDURE" DECTRI(SUB, DIAG, SUPER, N, AUX);  
"VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

SUB: <ARRAY IDENTIFIER>;  
"ARRAY" SUB[1: N - 1];  
ENTRY: THE SUBDIAGONAL OF THE GIVEN MATRIX T, SAY;  
T[I + 1, I] SHOULD BE GIVEN IN SUB[I], I = 1,  
..., N - 1;  
EXIT: SUPPOSE L DENOTES THE LOWER-BIDIAGONAL MATRIX, SUCH  
THAT LU = T, FOR SOME UPPER-BIDIAGONAL MATRIX U,  
WITH UNIT DIAGONAL ELEMENTS, THEN L[I + 1, I] WILL  
BE DELIVERED IN SUB[I], I = 1, ..., AUX[3] = 1;

DIAG: <ARRAY IDENTIFIER>;  
 "ARRAY" DIAG[1:N];  
 ENTRY: THE DIAGONAL OF T;  
 EXIT: L[I, I] WILL BE DELIVERED IN DIAG[I], I = 1, ..., AUX[3];

SUPER: <ARRAY IDENTIFIER>;  
 "ARRAY" SUPER[1:N - 1];  
 ENTRY: THE SUPERDIAGONAL OF T; T[I, I + 1] SHOULD BE GIVEN  
 IN SUPER[I], I = 1, ..., N - 1;  
 EXIT: U[I, I + 1] WILL BE DELIVERED IN SUPER[I], I = 1,  
 ..., AUX[3] - 1;

N: <ARITHMETICAL EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[2:5];  
 ENTRY :  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS, HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;

EXIT:  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED;  
 AUX[5]: IF AUX[3] = N, THEN AUX[5] WILL EQUAL THE INFINITY-  
 NORM OF THE MATRIX, ELSE AUX[5] IS SET EQUAL TO  
 THE VALUE OF THAT ELEMENT WHICH CAUSES THE  
 BREAKDOWN OF THE DECOMPOSITION.

PROCEDURES USED: NONE.

LANGUAGE: ALGOL 60.

#### METHOD AND PERFORMANCE:

THE METHOD USED IN DECTRI YIELDS A LOWER-BIDIAGONAL MATRIX L AND A  
 UNIT UPPER-BIDIAGONAL MATRIX U, SUCH THAT THE PRODUCT LU EQUALS THE  
 GIVEN TRIDIAGONAL MATRIX; THE PROCESS IS TERMINATED IN THE K-TH  
 STEP, IF THE MODULUS OF THE K-TH DIAGONAL ELEMENT IS SMALLER THAN A  
 CERTAIN SMALL VALUE, WHICH IS GIVEN BY AUX[2] MULTIPLIED BY THE  
 1-NORM OF THE K-TH ROW; IN THIS CASE AUX[3] WILL BE GIVEN THE VALUE  
 K - 1 AND AUX[5] WILL BE GIVEN THE VALUE OF THE K-TH DIAGONAL  
 ELEMENT.

EXAMPLE OF USE: SEE DECSOLTRI (SECTION 3.1.2.1.1.1.2.3).

SUBSECTION: DECTRIPIV.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:

```

"PROCEDURE" DECTRIPIV(SUB, DIAG, SUPER, N, AID, AUX, PIV);
"VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AID, AUX;
"BOOLEAN" "ARRAY" PIV;

```

THE MEANING OF THE FORMAL PARAMETERS IS:

```

SUB:   <ARRAY IDENTIFIER>;
       "ARRAY" SUB[1: N - 1];
ENTRY: THE SUBDIAGONAL OF THE GIVEN MATRIX T, SAY;
       T[I+1,I] SHOULD BE GIVEN IN SUB[I], I > 1, ..., N - 2
EXIT:  LET T' DENOTE THE MATRIX T WITH PERMUTED ROWS;
       SUPPOSE L DENOTES THE LOWER-BIDIAGONAL MATRIX, SUCH
       THAT LU = T', FOR SOME UNIT UPPER-TRIANGULAR MATRIX
       U, THEN L[I + 1, I] WILL BE DELIVERED IN SUB[I],
       I = 1, ..., AUX[3] - 1; NOTE THAT U HAS TWO
       GODIAGONALS, BECAUSE OF THE PARTIAL PIVOTING DURING
       THE DECOMPOSITION;

DIAG:  <ARRAY IDENTIFIER>;
       "ARRAY" DIAG[1: N];
ENTRY: THE DIAGONAL OF T;
EXIT:  L[I,I] WILL BE DELIVERED IN DIAG[I], I=1, ..., AUX[3];

SUPER: <ARRAY IDENTIFIER>;
       "ARRAY" SUPER[1: N - 1];
ENTRY: THE SUPERDIAGONAL OF T; T[I, I + 1] SHOULD BE GIVEN
       IN SUPER[I], I = 1, ..., N - 1;
EXIT:  U[I, I + 1] WILL BE DELIVERED IN SUPER[I], I = 1,
       ..., AUX[3] - 1;

N:     <ARITHMETICAL EXPRESSION>;
       THE ORDER OF THE MATRIX;

AID:   <ARRAY IDENTIFIER>;
       "ARRAY" AID[1: N - 2];
EXIT:  U[I, I+2] WILL BE DELIVERED IN AID[I], I=1, ..., AUX[3]-2;

AUX:   <ARRAY IDENTIFIER>;
       "ARRAY" AUX[2:5];
ENTRY:
AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS
       VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF
       THE MATRIX ELEMENTS, HOWEVER, IT SHOULD NOT BE
       CHOSEN SMALLER THAN THE MACHINE PRECISION;
EXIT:
AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED;
AUX[5]: IF AUX[3] = N, THEN AUX[5] WILL EQUAL THE INFINITY-
       NORM OF THE MATRIX, ELSE AUX[5] IS SET EQUAL TO
       THE VALUE OF THAT ELEMENT WHICH CAUSES THE
       BREAKDOWN OF THE DECOMPOSITION.

PIV:   <ARRAY IDENTIFIER>;
       "BOOLEAN""ARRAY" PIV[1 : N - 1];
       THE VALUE OF PIV[I] WILL BE TRUE IF THE I-TH AND (I + 1)-TH
       ROW ARE INTERCHANGED, I = 1, ..., MIN(AUX[3], N - 1), ELSE
       PIV[I] WILL BE FALSE.

```

SECTION 3.1.2.1.1.1.2.1

(JUNE 1974)

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PROCEDURES USED: NONE.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE METHOD USED IN DECTRIPIV YIELDS A LOWER-BIDIAGONAL MATRIX L AND A UNIT UPPER-TRIANGULAR MATRIX U WITH TWO CODIAGONALS, SUCH THAT THE PRODUCT LU EQUALS THE GIVEN TRIDIAGONAL MATRIX WITH PERMUTED ROWS; PARTIAL PIVOTING IS USED DURING THE TRIANGULAR DECOMPOSITION, I.E. THAT ELEMENT OF THE K-TH COLUMN OF L IS CHOSEN AS PIVOT IN THE K-TH STEP, WHOSE MODULUS DIVIDED BY THE 1-NORM OF THE CORRESPONDING ROW OF THE GIVEN MATRIX IS MAXIMAL; THE PROCESS IS TERMINATED IN THE K-TH STEP, IF THE MODULUS OF THE K-TH PIVOT ELEMENT IS LESS THAN A CERTAIN SMALL VALUE, WHICH IS GIVEN BY AUX[2] MULTIPLIED BY THE 1-NORM OF THE CORRESPONDING ROW; IN THIS CASE AUX[3] WILL BE GIVEN THE VALUE K - 1, AND AUX[5] WILL BE GIVEN THE VALUE OF THE K-TH PIVOT ELEMENT.

EXAMPLE OF USE: SEE SOLTRIPIV (SECTION 3.1.2.1.1.1.2.3).

SOURCE TEXTS:

```

"CODE" 34423;
"PROCEDURE" DECTRI(SUB, DIAG, SUPER, N, AUX);
"VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AUX;
"BEGIN" "INTEGER" I, N1;
  "REAL" D, R, S, U, NORM, NORM1, TOL;
  TOL:= AUX[2]; D:= DIAG[1]; R:= SUPER[1];
  NORM:= NORM1:= ABS(D) + ABS(R);
  "IF" ABS(D) <= NORM1 * TOL "THEN"
  "BEGIN" AUX[3]:= 0; AUX[5]:= D; "GOTO" EXIT "END";
  U:= SUPER[1]:= R / D; S:= SUB[1]; N1:= N - 1;
  "FOR" I:= 2 "STEP" 1 "UNTIL" N1 "DO"
  "BEGIN" D:= DIAG[I]; R:= SUPER[I];
    NORM1:= ABS(S) + ABS(D) + ABS(R);
    D:= DIAG[I]:= D - U * S;
    "IF" ABS(D) <= NORM1 * TOL "THEN"
    "BEGIN" AUX[3]:= I - 1; AUX[5]:= D; "GOTO" EXIT "END";
    U:= SUPER[I]:= R / D; S:= SUB[I];
    "IF" NORM1 > NORM "THEN" NORM:= NORM1
  "END";
  D:= DIAG[N]; NORM1:= ABS(D) + ABS(S);
  D:= DIAG[N]:= D - U * S;
  "IF" ABS(D) <= NORM1 * TOL "THEN"
  "BEGIN" AUX[3]:= N1; AUX[5]:= D; "GOTO" EXIT "END";
  "IF" NORM1 > NORM "THEN" NORM:= NORM1;
  AUX[3]:= N; AUX[5]:= NORM;
EXIT:
"END" DECTRI;
"EOP"

```

```

"CODE" 34426;
"PROCEDURE" DECTRIPIV(SUB, DIAG, SUPER, N, AID, AUX, PIV);
"VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AID, AUX;
"BOOLEAN" "ARRAY" PIV;
"BEGIN" "INTEGER" I, I1, N1, N2;
"REAL" D, R, S, U, T, Q, V, W, NORM, NORM1, NORM2, TOL;
TOL:= AUX[2]; D:= DIAG[1]; R:= SUPER[1];
NORM:= NORM2:= ABS(D) + ABS(R); N2:= N - 2;
"FOR" I:= 1 "STEP" 1 "UNTIL" N2 "DO"
"BEGIN" I1:= I + 1; S:= SUB[I]; T:= DIAG[I1]; Q:= SUPER[I1];
NORM1:= NORM2; NORM2:= ABS(S) + ABS(T) + ABS(Q);
"IF" NORM2 > NORM "THEN" NORM:= NORM2;
"IF" ABS(D) * NORM2 < ABS(S) * NORM1 "THEN"
"BEGIN" "IF" ABS(S) <= TOL * NORM2 "THEN"
"BEGIN" AUX[3]:= I - 1; AUX[5]:= S; "GOTO" EXIT "END";
DIAG[I]:= S; U:= SUPER[I]:= T / S;
V:= AID[I]:= Q / S; SUB[I]:= D;
W:= SUPER[I1]:= -V * D; D:= DIAG[I1]:= R - U * D;
R:= W; NORM2:= NORM1; PIV[I]:= "TRUE"
"END" "ELSE"
"BEGIN" "IF" ABS(D) <= TOL * NORM1 "THEN"
"BEGIN" AUX[3]:= I - 1; AUX[5]:= D; "GOTO" EXIT "END";
U:= SUPER[I]:= R / D; D:= DIAG[I1]:= T - U * S;
AID[I]:= 0; PIV[I]:= "FALSE"; R:= Q
"END"
"END";
N1:= N - 1; S:= SUB[N1]; T:= DIAG[N]; NORM1:= NORM2;
NORM2:= ABS(S) + ABS(T); "IF" NORM2 > NORM "THEN" NORM:= NORM2;
"IF" ABS(D) * NORM2 < ABS(S) * NORM1 "THEN"
"BEGIN" "IF" ABS(S) <= TOL * NORM2 "THEN"
"BEGIN" AUX[3]:= N2; AUX[5]:= S; "GOTO" EXIT "END";
DIAG[N1]:= S; U:= SUPER[N1]:= T / S; SUB[N1]:= D;
D:= DIAG[N]:= R - U * D; NORM2:= NORM1; PIV[N1]:= "TRUE"
"END" "ELSE"
"BEGIN" "IF" ABS(D) <= TOL * NORM1 "THEN"
"BEGIN" AUX[3]:= N2; AUX[5]:= D; "GOTO" EXIT "END";
U:= SUPER[N1]:= R / D; D:= DIAG[N]:= T - U * S;
PIV[N1]:= "FALSE"
"END";
"IF" ABS(D) <= TOL * NORM2 "THEN"
"BEGIN" AUX[3]:= N1; AUX[5]:= D; "GOTO" EXIT "END";
AUX[3]:= N; AUX[5]:= NORM;
EXIT;
"END" DECTRIPIV;
"EOP"
    
```



SECTION 3.1.2.1.1.1.2.3

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PAGE 1

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## BRIEF DESCRIPTION:

THIS SECTION CONTAINS FOUR PROCEDURES FOR SOLVING A SYSTEM OF LINEAR EQUATIONS WITH A TRIDIAGONAL MATRIX; SOLTRI CALCULATES A SOLUTION BY FORWARD AND BACK SUBSTITUTION IF THE TRIANGULAR DECOMPOSED FORM AS DELIVERED BY DECTRI IS GIVEN. DECSOLTRI PERFORMS THE TRIANGULAR DECOMPOSITION OF THE GIVEN MATRIX ( NOT USING ANY PIVOTING STRATEGY DURING THE PROCESS ) AND CALCULATES THE SOLUTION BY FORWARD AND BACK SUBSTITUTION. SOLTRIPIV CALCULATES A SOLUTION BY FORWARD AND BACK SUBSTITUTION, IF THE TRIANGULAR DECOMPOSED FORM AS DELIVERED BY DECTRIPIV IS GIVEN. DECSOLTRIPIV PERFORMS THE TRIANGULAR DECOMPOSITION OF THE GIVEN MATRIX ( USING PARTIAL PIVOTING ) AND CALCULATES THE SOLUTION BY FORWARD AND BACK SUBSTITUTION.

## KEYWORDS:

ALGEBRAIC EQUATIONS,  
LINEAR SYSTEMS,  
TRIDIAGONAL MATRIX,  
FORWARD AND BACK SUBSTITUTION.

SUBSECTION: SOLTRI.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" SOLTRI(SUB, DIAG, SUPER, N, B);  
 "VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

SUB: <ARRAY IDENTIFIER>;  
 "ARRAY" SUB[1, N - 1];  
 ENTRY : THE SUBDIAGONAL OF THE  
 LOWER-BIDIAGONAL MATRIX, AS DELIVERED BY DECTRI (SECTION  
 3.1.2.1.1.1.2.1);  
 DIAG: <ARRAY IDENTIFIER>;  
 "ARRAY" DIAG[1:N];  
 ENTRY : THE DIAGONAL OF THE LOWER-  
 BIDIAGONAL MATRIX, AS DELIVERED BY DECTRI;  
 SUPER: <ARRAY IDENTIFIER>;  
 "ARRAY" SUPER[1; N - 1];  
 ENTRY : THE SUPERDIAGONAL OF THE  
 UPPER-BIDIAGONAL MATRIX AS DELIVERED BY DECTRI;  
 N: <ARITHMETICAL EXPRESSION>;  
 THE ORDER OF THE MATRIX;  
 B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: THE CALCULATED SOLUTION OF THE LINEAR SYSTEM.

PROCEDURES USED: NONE.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SOLTRI CALCULATES THE SOLUTION OF A LINEAR SYSTEM WITH A TRIDIAGONAL MATRIX, WITH FORWARD AND BACK SUBSTITUTION; THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX, AS PRODUCED BY DECTRI (SECTION 3.1.2.1.1.1.2.1), SHOULD BE GIVEN; ONE CALL OF DECTRI FOLLOWED BY SEVERAL CALLS OF SOLTRI MAY BE USED TO SOLVE SEVERAL LINEAR SYSTEMS HAVING THE SAME TRIDIAGONAL MATRIX, BUT DIFFERENT RIGHT-HAND SIDES.

EXAMPLE OF USE: SEE DECSOLTRI (THIS SECTION).

SUBSECTION: DECSOLTRI.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:

"PROCEDURE" DECSOLTRI(SUB, DIAG, SUPER, N, AUX, B);

"VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

SUB: <ARRAY IDENTIFIER>;

"ARRAY" SUB[1: N - 1];

ENTRY: THE SUBDIAGONAL OF THE GIVEN MATRIX T, SAY;  
 $T[I + 1, I]$  SHOULD BE GIVEN IN SUB[I],  $I = 1, \dots, N - 1$ ;

EXIT: SUPPOSE L DENOTES THE LOWER-BIDIAGONAL MATRIX, SUCH  
 THAT  $LU = T$ , FOR SOME UPPER-BIDIAGONAL MATRIX U,  
 WITH UNIT DIAGONAL ELEMENTS, THEN  $L[I + 1, I]$  WILL  
 BE DELIVERED IN SUB[I],  $I = 1, \dots, AUX[3] - 1$ ;

DIAG: <ARRAY IDENTIFIER>;

"ARRAY" DIAG[1: N];

ENTRY: THE DIAGONAL OF T;

EXIT:  $L[I, I]$  WILL BE DELIVERED IN DIAG[I],  $I = 1, \dots, \dots, AUX[3]$ ;

SUPER: <ARRAY IDENTIFIER>;

"ARRAY" SUPER[1: N - 1];

ENTRY: THE SUPERDIAGONAL OF T;  $T[I, I + 1]$  SHOULD BE GIVEN  
 IN SUPER[I],  $I = 1, \dots, N - 1$ ;

EXIT:  $U[I, I + 1]$  WILL BE DELIVERED IN SUPER[I],  $I = 1, \dots, AUX[3] - 1$ ;

N: <ARITHMETICAL EXPRESSION>;

THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;

"ARRAY" AUX[2:5];

ENTRY :

AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS, HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;

EXIT :

AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED;

AUX[5]: IF  $AUX[3] = N$ , THEN AUX[5] WILL EQUAL THE INFINITY-  
 NORM OF THE MATRIX (SEE SECTION 3.1.2.1.1.1.2.1,  
 SUBSECTION DECTRI);

B: <ARRAY IDENTIFIER>;

"ARRAY" B[1:N];

ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;

EXIT: IF  $AUX[3] = N$ , THEN THE SOLUTION OF THE LINEAR  
 SYSTEM IS OVERWRITTEN ON B, ELSE B REMAINS  
 UNALTERED.

PROCEDURES USED:

DECTRI = CP34423,  
SOLTRI = CP34424.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

DECSOLTRI CALCULATES THE SOLUTION OF A LINEAR SYSTEM WITH A TRIDIAGONAL MATRIX; THE TRIANGULAR DECOMPOSITION IS DONE BY CALLING DECTRI (SECTION 3.1.2.1.1.1.2.1) AND THE FORWARD AND BACK SUBSTITUTION BY CALLING SOLTRI (THIS SECTION); IF AUX[3] < N, THEN THE EFFECT OF DECSOLTRI IS MERELY THAT OF DECTRI.

EXAMPLE OF USE:

LET T BE A TRIDIAGONAL MATRIX WITH SUBDIAGONAL AND SUPERDIAGONAL ELEMENTS  $I * 2$  AND  $I$  RESPECTIVELY ( $I = 1, \dots, N - 1$ ), AND DIAGONAL ELEMENTS  $I + 10$  ( $I = 1, \dots, N$ ); LET B BE THE SECOND COLUMN OF T; THEN THE SOLUTION OF THE LINEAR SYSTEM  $TX = B$  IS GIVEN BY THE SECOND UNIT VECTOR; BY THE FOLLOWING PROGRAM WE MAY SOLVE THIS SYSTEM AND PRINT THE ERROR IN THE CALCULATED SOLUTION.

```
"BEGIN"
  "PROCEDURE" DECSOLTRI(L, D, U, N, A, B); "CODE" 34425;
  "REAL" "PROCEDURE" VECVEC(L, U, S, A, B); "CODE" 34010;
  "INTEGER" I;
  "ARRAY" D, SUB, SUPER, B[1:30], AUX[2:5];
  "FOR" I:= 1 "STEP" 1 "UNTIL" 30 "DO"
    "BEGIN" SUB[I]:= I * 2; SUPER[I]:= I; D[I]:= I + 10;
      B[I]:= 0
    "END"; B[1]:= 1; B[2]:= 12; B[3]:= 4;
  AUX[2]:= "-14";
  DECSOLTRI(SUB, D, SUPER, 30, AUX, B);
  OUTPUT(71, "( "/" ("AUX[3] AND AUX[5]:")", 2( /, N) )",
  AUX[3], AUX[5]);
  B[2]:= B[2] - 1;
  OUTPUT(71, "( "/" ("ERROR IN THE SOLUTION: ")", N) ",
  Sqrt(VECVEC(1, 30, 0, B, B)))
"END"
```

RESULTS:

AUX[3] AND AUX[5]:  
+3.0000000000000000"+001  
+1.2400000000000000"+002

ERROR IN THE SOLUTION: +0.0000000000000000"+000

SUBSECTION: SOLTRIPIV.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:

"PROCEDURE" SOLTRIPIV(SUB, DIAG, SUPER, N, AID, PIV, B);  
 "VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AID, B;  
 "BOOLEAN" "ARRAY" PIV;

THE MEANING OF THE FORMAL PARAMETERS IS:

SUB: <ARRAY IDENTIFIER>;  
 "ARRAY" SUB[1, N - 1];  
 ENTRY: THE SUBDIAGONAL OF THE  
 LOWER-BIDIAGONAL MATRIX, AS DELIVERED BY DECTRIPIV (SECTION  
 3.1.2.1.1.1.2.1);

DIAG: <ARRAY IDENTIFIER>;  
 "ARRAY" DIAG[1:N];  
 ENTRY: THE DIAGONAL OF THE LOWER-  
 BIDIAGONAL MATRIX, AS DELIVERED BY DECTRIPIV;

SUPER: <ARRAY IDENTIFIER>;  
 "ARRAY" SUPER[1: N - 1];  
 ENTRY: THE FIRST CODIAGONAL OF  
 THE UPPER-TRIANGULAR MATRIX AS DELIVERED BY DECTRIPIV;

N: <ARITHMETICAL EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AID: <ARRAY IDENTIFIER>;  
 "ARRAY" AID[1: N - 2];  
 ENTRY: THE SECOND CODIAGONAL OF  
 THE UPPER-TRIANGULAR MATRIX AS DELIVERED BY DECTRIPIV;

PIV: <ARRAY IDENTIFIER>;  
 "BOOLEAN" "ARRAY" PIV[1: N-1];  
 ENTRY: THE PIVOT-  
 INFORMATION AS DELIVERED BY DECTRIPIV;

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: THE CALCULATED SOLUTION OF THE LINEAR SYSTEM.

PROCEDURES USED: NONE.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SOLTRIPIV CALCULATES THE SOLUTION OF A LINEAR SYSTEM WITH A TRIDIAGONAL MATRIX, WITH FORWARD AND BACK SUBSTITUTION; THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX, AS PRODUCED BY DECTRIPIV (SECTION 3.1.2.1.1.1.2.1), SHOULD BE GIVEN; ONE CALL OF DECTRIPIV FOLLOWED BY SEVERAL CALLS OF SOLTRIPIV MAY BE USED TO SOLVE SEVERAL LINEAR SYSTEMS HAVING THE SAME TRIDIAGONAL MATRIX, BUT DIFFERENT RIGHT-HAND SIDES.

## EXAMPLE OF USE:

LET T BE THE MATRIX AS GIVEN IN THE EXAMPLE OF USE OF DECSOLTRI (THIS SECTION) AND LET B1 AND B2 BE THE SECOND AND THIRD COLUMN OF T, THEN THE SOLUTIONS OF THE LINEAR SYSTEMS  $TX = B1$  AND  $TX = B2$  ARE GIVEN BY THE SECOND AND THIRD UNIT VECTOR RESPECTIVELY; IN THE FOLLOWING PROGRAM THESE SYSTEMS ARE SOLVED AND THE ERRORS IN THE CALCULATED SOLUTIONS ARE PRINTED.

```

"BEGIN"
  "PROCEDURE" DECTRIPIV(L, D, U, N, A, AX, P); "CODE" 34426;
  "PROCEDURE" SOLTRIPIV(L, D, U, N, A, P, B); "CODE" 34427;
  "REAL" "PROCEDURE" VECVEC(L, U, S, A, B); "CODE" 34010;
  "INTEGER" I;
  "ARRAY" D, SUB, SUPER, AID, B1, B2[1:30], AUX[2:5];
  "BOOLEAN" "ARRAY" PIV[1:29];
  "FOR" I:= 1 "STEP" 1 "UNTIL" 30 "DO"
  "BEGIN" SUB[I]:= I * 2; SUPER[I]:= I; D[I]:= I + 10;
    B1[I]:= B2[I]:= 0
  "END"; B1[1]:= 1; B1[2]:= 12; B1[3]:= 4;
  B2[2]:= 2; B2[3]:= 13; B2[4]:= 6;
  AUX[2]:= -14;
  DECTRIPIV(SUB, D, SUPER, 30, AID, AUX, PIV);
  SOLTRIPIV(SUB, D, SUPER, 30, AID, PIV, B1);
  SOLTRIPIV(SUB, D, SUPER, 30, AID, PIV, B2);
  OUTPUT(71, "("/,"("AUX[3] AND AUX[5];")",2(/,N)"),
  AUX[3], AUX[5]);
  B1[2]:= B1[2] - 1; B2[3]:= B2[3] - 1;
  OUTPUT(71, "("//,"("ERROR IN B1: ")",N,"("ERROR IN B2: ")",N)"),
  SQRT(VECVEC(1, 30, 0, B1, B1)), SQRT(VECVEC(1, 30, 0, B2, B2)))
"END"

```

## RESULTS:

```

AUX[3] AND AUX[5]:
+3,0000000000000000"+001
+1,2400000000000000"+002

```

```

ERROR IN B1: +0,0000000000000000"+000
ERROR IN B2: +0,0000000000000000"+000

```

## SUBSECTION: DECSOLTRIPV.

## CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" DECSOLTRIPV(SUB, DIAG, SUPER, N, AUX, B);  
 "VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

SUB: <ARRAY IDENTIFIER>;  
 "ARRAY" SUB[1: N - 1];  
 ENTRY: THE SUBDIAGONAL OF THE GIVEN MATRIX T, SAY;  
 T[I + 1, I] SHOULD BE GIVEN IN SUB[I], I = 1,  
 ..., N - 1;  
 EXIT: THE ELEMENTS OF SUB WILL BE OVERWRITTEN;

DIAG: <ARRAY IDENTIFIER>;  
 "ARRAY" DIAG[1: N];  
 ENTRY: THE DIAGONAL OF T;  
 EXIT: THE ELEMENTS OF DIAG WILL BE OVERWRITTEN;

SUPER: <ARRAY IDENTIFIER>;  
 "ARRAY" SUPER[1: N - 1];  
 ENTRY: THE SUPERDIAGONAL OF T; T[I, I + 1] SHOULD BE GIVEN  
 IN SUPER[I], I = 1, ..., N - 1;  
 EXIT: THE ELEMENTS OF SUPER WILL BE OVERWRITTEN;

N: <ARITHMETICAL EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[2:5];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS, HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 EXIT:  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED;  
 AUX[5]: IF AUX[3] = N, THEN AUX[5] WILL EQUAL THE INFINITY-  
 NORM OF THE MATRIX (SEE SECTION 3.1.2.1.1.1.2.1.,  
 SUBSECTION DECTRIPIV);

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1: N];  
 ENTRY: THE RIGHT-HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: IF AUX[3] = N, THEN THE SOLUTION OF THE LINEAR  
 SYSTEM WILL BE OVERWRITTEN ON B, ELSE B WILL REMAIN  
 UNALTERED.

PROCEDURES USED: NONE.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: ONE AUXILIARY ARRAY OF TYPE BOOLEAN AND ORDER N IS DECLARED IN DECSOLTRIPV;

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

ONE CALL OF DECSOLTRIPV IS EQUIVALENT WITH CALLING CONSECUTIVELY DECTRIPIV (SECTION 3.1.2.1.1.1.2.1) AND SOLTRIPV (THIS SECTION); HOWEVER, DECSOLTRIPV DOES NOT MAKE USE OF DECTRIPIV AND SOLTRIPV, TO SAVE MEMORY SPACE AND TIME; THIS IS ONLY TRUE IN THE CASE THAT LINEAR SYSTEMS WITH DIFFERENT MATRICES HAVE TO BE SOLVED; IF  $AUX[3] < N$  THEN DECSOLTRIPV IS TERMINATED PREMATURELY (SEE DECTRIPIV IN SECTION 3.1.2.1.1.1.2.1).

EXAMPLE OF USE:

THE SAME LINEAR SYSTEM AS GIVEN IN THE EXAMPLE OF USE OF DECSOLTRI MAY BE SOLVED WITH DECSOLTRIPV BY THE FOLLOWING PROGRAM:

```

"BEGIN"
  "PROCEDURE" DECSOLTRIPV(L, D, U, N, A, B); "CODE" 34428;
  "REAL" "PROCEDURE" VECVEC(L, U, S, A, B); "CODE" 34010;
  "INTEGER" I;
  "ARRAY" D, SUB, SUPER, B[1:30], AUX[2:5];
  "FOR" I:= 1 "STEP" 1 "UNTIL" 30 "DO"
    "BEGIN" SUB[I]:= I * 2; SUPER[I]:= I; D[I]:= I + 10;
      B[I]:= 0
    "END"; B[1]:= 1; B[2]:= 12; B[3]:= 4;
  AUX[2]:= "-14";
  DECSOLTRIPV(SUB, D, SUPER, 30, AUX, B);
  OUTPUT(71, "("/,"("AUX[3] AND AUX[5]:")",2(/,N)"",
  AUX[3], AUX[5]);
  B[2]:= B[2] - 1;
  OUTPUT(71, "("//>("ERROR IN THE SOLUTION: ")", N)"",
  Sqrt(VECVEC(1, 30, 0, B, B)))
"END"

```

RESULTS:

```

AUX[3] AND AUX[5]:
+3.0000000000000000"+001
+1.2400000000000000"+002

```

```

ERROR IN THE SOLUTION: +0.0000000000000000"+000

```



## SOURCE TEXTS:

```

"CODE" 34424;
"PROCEDURE" SOLTRI(SUB, DIAG, SUPER, N, B);
"VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, B;
"BEGIN" "INTEGER" I;
    "REAL" R;
    R:= B[1]:= B[1] / DIAG[1];
    "FOR" I:= 2 "STEP" 1 "UNTIL" N "DO"
    R:= B[I]:= (B[I] - SUB[I - 1] * R) / DIAG[I];
    "FOR" I:= N - 1 "STEP" -1 "UNTIL" 1 "DO"
    R:= B[I] := B[I] - SUPER[I] * R
"END" SOLTRI;
    "EOP"
    
```

```

"CODE" 34425;
"PROCEDURE" DECSOLTRI(SUB, DIAG, SUPER, N, AUX, B);
"VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AUX, B;
"BEGIN" "PROCEDURE" DECTRI(SUB, DIAG, SUPER, N, AUX); "CODE" 34423;
    "PROCEDURE" SOLTRI(SUB, DIAG, SUPER, N, B); "CODE" 34424;
    DECTRI(SUB, DIAG, SUPER, N, AUX); "IF" AUX[3]= N "THEN"
    SOLTRI(SUB, DIAG, SUPER, N, B)
"END" DECSOLTRI;
    "EOP"
    
```

```

"CODE" 34427;
"PROCEDURE" SOLTRIPIV(SUB, DIAG, SUPER, N, AID, PIV, B);
"VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AID, B;
"BOOLEAN" "ARRAY" PIV;
"BEGIN" "INTEGER" I, N1;
    "REAL" BI, BI1, R, S, T;
    N1:= N - 1;
    "FOR" I:= 1 "STEP" 1 "UNTIL" N1 "DO"
    "BEGIN" "IF" PIV[I] "THEN"
        "BEGIN" BI:= B[I+1]; BI1:= B[I] "END"
        "ELSE"
            "BEGIN" BI:= B[I]; BI1:= B[I+1] "END";
        R:= B[I]:= BI / DIAG[I];
        B[I+1]:= BI1 - SUB[I] * R
    "END";
    R:= B[N]:= B[N] / DIAG[N];
    T:= B[N1]:= B[N1] - SUPER[N1] * R;
    "FOR" I:= N - 2 "STEP" -1 "UNTIL" 1 "DO"
    "BEGIN" S:= R; R:= T; T:= B[I]:= B[I] - SUPER[I] * R -
        ("IF" PIV[I] "THEN" AID[I] * S "ELSE" 0)
    "END"
"END" SOLTRIPIV;
    "EOP"
    
```

```

"CODE" 34428;
"PROCEDURE" DECSOLTRIPIV(SUB, DIAG, SUPER, N, AUX, B);
"VALUE" N; "INTEGER" N; "ARRAY" SUB, DIAG, SUPER, AUX, B;
"BEGIN" "INTEGER" I, I1, N1, N2;
"REAL" D, R, S, U, T, Q, V, W, NORM, NORM1, NORM2, TOL,
BI, BI1, BI2;
"BOOLEAN" "ARRAY" PIV[1:N];
TOL:= AUX[2]; D:= DIAG[1]; R:= SUPER[1]; BI:= B[1];
NORM:= NORM2:= ABS(D) + ABS(R); N2:= N - 2;
"FOR" I:= 1 "STEP" 1 "UNTIL" N2 "DO"
"BEGIN" I1:= I + 1; S:= SUB[I]; T:= DIAG[I1]; Q:= SUPER[I1];
BI1:= B[I1];
NORM1:= NORM2; NORM2:= ABS(S) + ABS(T) + ABS(Q);
"IF" NORM2 > NORM "THEN" NORM:= NORM2;
"IF" ABS(D) * NORM2 < ABS(S) * NORM1 "THEN"
"BEGIN" "IF" ABS(S) <= TOL * NORM2 "THEN"
"BEGIN" AUX[3]:= I - 1; AUX[5]:= S; "GOTO" EXIT "END";
U:= SUPER[I]:= T / S; BI1:= B[I]:= BI / S;
BI:= BI - BI1 * D; V:= SUB[I]:= Q / S;
W:= SUPER[I1]:= -V * D; D:= DIAG[I1]:= R - U * D;
R:= W; NORM2:= NORM1; PIV[I]:= "TRUE"
"END" "ELSE"
"BEGIN" "IF" ABS(D) <= TOL * NORM1 "THEN"
"BEGIN" AUX[3]:= I - 1; AUX[5]:= D; "GOTO" EXIT "END";
U:= SUPER[I]:= R / D; BI:= B[I]:= BI / D;
BI:= BI - BI * S; D:= DIAG[I1]:= T - U * S;
PIV[I]:= "FALSE"; R:= Q
"END"
"END";
N1:= N - 1; S:= SUB[N1]; T:= DIAG[N]; NORM1:= NORM2; BI1:= B[N];
NORM2:= ABS(S) + ABS(T); "IF" NORM2 > NORM "THEN" NORM:= NORM2;
"IF" ABS(D) * NORM2 < ABS(S) * NORM1 "THEN"
"BEGIN" "IF" ABS(S) <= TOL * NORM2 "THEN"
"BEGIN" AUX[3]:= N2; AUX[5]:= S; "GOTO" EXIT "END";
U:= SUPER[N1]:= T / S; BI1:= B[N1]:= BI / S;
BI:= BI - BI1 * D; D:= R - U * D; NORM2:= NORM1
"END" "ELSE"
"BEGIN" "IF" ABS(D) <= TOL * NORM1 "THEN"
"BEGIN" AUX[3]:= N2; AUX[5]:= D; "GOTO" EXIT "END";
U:= SUPER[N1]:= R / D; BI:= B[N1]:= BI / D;
BI:= BI - BI * S; D:= T - U * S
"END";
"IF" ABS(D) <= TOL * NORM2 "THEN"
"BEGIN" AUX[3]:= N1; AUX[5]:= D; "GOTO" EXIT "END";
AUX[3]:= N; AUX[5]:= NORM;
BI1:= B[N]:= BI / D; BI:= B[N1]:= B[N1] - SUPER[N1] * BI1;
"FOR" I:= N - 2 "STEP" -1 "UNTIL" 1 "DO"
"BEGIN" BI2:= BI1; BI1:= BI;
BI:= B[I]:= B[I] - SUPER[I] * BI1 -
("IF" PIV[I] "THEN" SUB[I] * BI2 "ELSE" 0)
"END";
EXIT;
"END" DECSOLTRIPIV;
"EOP"
    
```

SECTION 3.1.2.1.1.2.1.1

(DECEMBER 1975)

PAGE 1

AUTHOR : T.J. DEKKER.  
 CONTRIBUTOR : J. KOK.  
 INSTITUTE : MATHEMATICAL CENTRE.  
 RECEIVED : 731001.

BRIEF DESCRIPTION :  
 THIS SECTION CONTAINS THE PROCEDURE CHLDECBND  
 FOR THE CHOLESKY DECOMPOSITION OF A SYMMETRIC POSITIVE DEFINITE  
 BAND MATRIX.

KEYWORDS :  
 LINEAR EQUATIONS,  
 CHOLESKY DECOMPOSITION,  
 SYMMETRIC POSITIVE DEFINITE MATRIX,  
 BAND MATRIX.

## CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :  
 "PROCEDURE" CHLDECBND(A, N, W, AUX); "VALUE" N, W; "INTEGER" N, W;  
 "ARRAY" A, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS :

A : <ARRAY IDENTIFIER>;  
 "ARRAY" A[1 : W \* (N - 1) + N];  
 ENTRY : A CONTAINS COLUMNWISE (I.E. THE (I,J)-TH  
 ELEMENT OF THE MATRIX IS A[(J-1)\*W+I], J=1,...,N,  
 I=MAX(1,J-W),...,J) THE UPPER-TRIANGULAR BAND  
 ELEMENTS OF THE SYMMETRIC BAND MATRIX;  
 EXIT : THE BAND ELEMENTS OF THE CHOLESKY  
 MATRIX, WHICH IS AN UPPER-TRIANGULAR BAND MATRIX WITH  
 W SUPERDIAGONALS, ARE DELIVERED COLUMNWISE IN A;  
 N : <ARITHMETIC EXPRESSION>;  
 ORDER OF THE BAND MATRIX;  
 W : <ARITHMETIC EXPRESSION>;  
 NUMBER OF SUPERDIAGONALS OF THE MATRIX;  
 AUX : <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[2 : 3];  
 ENTRY : AUX[2] IS A RELATIVE TOLERANCE TO CONTROL THE  
 CALCULATION OF THE DIAGONAL ELEMENTS OF THE  
 CHOLESKY MATRIX (SEE METHOD AND PERFORMANCE);  
 NORMAL EXIT :  
 AUX[3] = N;  
 ABNORMAL EXIT :  
 AUX[3] = K - 1, WHERE K IS THE INDEX OF THE DIAGONAL  
 ELEMENT OF THE CHOLESKY MATRIX THAT CANNOT BE  
 CALCULATED.

SECTION 3.1.2.1.1.2.1.1

(JUNE 1974)

PAGE 2

## PROCEDURES USED :

VECVEC = CP34010.

## RUNNING TIME :

(C1 \* W + C2) \* W \* N;  
THE CONSTANTS C1 AND C2 DEPEND UPON THE  
ARITHMETIC OF THE COMPUTER.

LANGUAGE : ALGOL 60.

## METHOD AND PERFORMANCE :

CHLDECBND PERFORMS THE CHOLESKY DECOMPOSITION OF A SYMMETRIC POSITIVE DEFINITE MATRIX, WHOSE NON-ZERO ELEMENTS ARE IN BAND FORM, AND WHOSE UPPER-TRIANGULAR BAND ELEMENTS ARE STORED COLUMNWISE IN IONAL ARRAY.

THE METHOD USED IS CHOLESKY'S SQUARE ROOT METHOD. IF THE GIVEN MATRIX IS POSITIVE DEFINITE, THEN THIS METHOD YIELDS AN UPPER-TRIANGULAR BAND MATRIX, THE CHOLESKY MATRIX. THE NUMBER OF NON-ZERO SUPERDIAGONALS OF THE GIVEN MATRIX AND ITS CHOLESKY MATRIX ARE EQUAL. THE PROCESS IS COMPLETED IN N STAGES, AT EACH STAGE PRODUCING A ROW OF THE CHOLESKY MATRIX. HOWEVER, THE PROCESS IS DISCONTINUED IF AT SOME STAGE, SAY K, THE K-TH DIAGONAL ELEMENT OF THE GIVEN MATRIX MINUS THE SUM OF SQUARES OF THE SUPERDIAGONAL ELEMENTS OF THE K-TH COLUMN OF THE CHOLESKY MATRIX (THE SQUARE ROOT OF THIS QUANTITY BEING THE K-TH DIAGONAL ELEMENT OF THE CHOLESKY MATRIX) IS EITHER NEGATIVE OR LESS THAN A GIVEN RELATIVE TOLERANCE (AUX[2]) TIMES THE MAXIMAL DIAGONAL ELEMENT OF THE GIVEN MATRIX. IN THIS CASE THE GIVEN MATRIX, POSSIBLY MODIFIED BY ROUNDING ERRORS, IS NOT POSITIVE DEFINITE. THIS IS INDICATED IN AUX[3], BY WHICH THE VALUE K - 1 IS DELIVERED. IF THE DECOMPOSITION IS CARRIED OUT FULLY, AUX[3] BECOMES N. THE PROCEDURE DELIVERS THE BAND ELEMENTS OF THE CHOLESKY MATRIX. SEE ALSO REF [1], SECTION 222.

## REFERENCE :

- [1] DEKKER, T.J. :  
ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 1,  
MC TRACT 22, 1968, MATHEMATISCH CENTRUM, AMSTERDAM.

## EXAMPLE OF USE :

SEE EXAMPLE OF USE OF CHLSOLBND.

## SOURCE TEXT(S) :

```

"CODE" 34330;
"PROCEDURE" CHLDECBND(A, N, W, AUX); "VALUE" N, W; "INTEGER" N, W;
"ARRAY" A, AUX;
"BEGIN" "INTEGER" J, K, JMAX, KK, KJ, W1, START;
"REAL" R, EPS, MAX;
"REAL" "PROCEDURE" VECVEC(L, U, S, A, B); "CODE" 34010;
MAX:= 0; KK:= - W; W1:= W + 1;
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" KK:= KK + W1; "IF" A[KK] > MAX "THEN" MAX:= A[KK] "END";
JMAX:= W; W1:= W + 1; KK:= - W; EPS:= AUX[2] * MAX;
"FOR" K:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" "IF" K + W > N "THEN" JMAX:= JMAX - 1; KK:= KK + W1;
START:= KK - K + 1;
R:= A[KK] - VECVEC("IF" K <= W1 "THEN" START "ELSE" KK - W,
KK - 1, 0, A, A); "IF" R <= EPS "THEN"
"BEGIN" AUX[3]:= K - 1; "GO TO" END "END";
A[KK]:= R:= SQRT(R); KJ:= KK;
"FOR" J:= 1 "STEP" 1 "UNTIL" JMAX "DO"
"BEGIN" KJ:= KJ + W;
A[KJ]:= (A[KJ] - VECVEC("IF" K + J <= W1 "THEN" START
"ELSE" KK - W + J, KK - 1, KJ - KK, A, A)) / R
"END"
"END";
AUX[3]:= N;
END;
"END" CHLDECBND;
"EQP"

```

SECTION 3.1.2.1.1.2.1.2 (JUNE 1974)

PAGE 1

CONTRIBUTOR : J. KOK.

INSTITUTE : MATHEMATICAL CENTRE.

RECEIVED : 731001.

BRIEF DESCRIPTION :

THIS SECTION CONTAINS ONE PROCEDURE, CHLDETERMBND, FOR THE CALCULATION OF THE DETERMINANT OF A SYMMETRIC POSITIVE DEFINITE BAND MATRIX.

KEY WORDS :

DETERMINANT,  
SYMMETRIC POSITIVE DEFINITE MATRIX,  
BAND MATRIX.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"REAL" "PROCEDURE" CHLDETERMBND(A, N, W); "VALUE" N, W;  
"INTEGER" N, W; "ARRAY" A;

CHLDETERMBND DELIVERS THE DETERMINANT OF THE SYMMETRIC POSITIVE DEFINITE BAND MATRIX WHOSE CHOLESKY MATRIX IS STORED IN A.

THE MEANING OF THE FORMAL PARAMETERS IS :

A, N, W : SEE CALLING SEQUENCE OF CHLDECBND  
(SECTION 3.1.2.1.1.2.1.1.);  
THE CONTENTS OF A ARE AS PRODUCED BY CHLDECBND OR  
CHLDECSOLBND (SECTION 3.1.2.1.1.2.1.3.).

PROCEDURES USED : NONE.

RUNNING TIME : PROPORTIONAL TO N.

LANGUAGE : ALGOL 60.

## METHOD AND PERFORMANCE :

CHLDETERMBND CAN BE CALLED AFTER CHLDECBND OR CHLDECSOLBND ONLY IF  
 THE CHOLESKY DECOMPOSITION WAS SUCCESSFUL, I.E. IF  
 AUX[3] = N.  
 THE FUNCTION VALUE OF CHLDETERMBND IS THE SQUARE OF THE DETERMINANT  
 OF THE CHOLESKY MATRIX.  
 CHLDETERMBND SHOULD NOT BE CALLED WHEN OVERFLOW CAN BE EXPECTED.

## EXAMPLE OF USE :

SEE EXAMPLES OF USE OF CHLSOLBND AND CHLDECSOLBND.

## SOURCE TEXT(S) :

```

"CODE" 34331;
"REAL" "PROCEDURE" CHLDETERMBND(A, N, W); "VALUE" N, W; "INTEGER" N, W;
"ARRAY" A;
"BEGIN" "INTEGER" J, KK, W1; "REAL" P;
      W1 := W + 1; KK := - W; P := 1;
      "FOR" J := 1 "STEP" 1 "UNTIL" N "DO"
        "BEGIN" KK := KK + W1; P := A[KK] * P "END";
      CHLDETERMBND := P * P
"END" CHLDETERMBND;
"EOB"
  
```

SECTION 3.1.2.1.1.2.1.3

(DECEMBER 1975)

PAGE 1

AUTHOR : T.J. DEKKER.

CONTRIBUTOR : J. KOK.

INSTITUTE : MATHEMATICAL CENTRE.

RECEIVED : 731001.

BRIEF DESCRIPTION :

THIS SECTION CONTAINS TWO PROCEDURES.

A) CHLSOLBND, FOR THE SOLUTION OF ONE OR MORE SYSTEMS OF LINEAR EQUATIONS WITH THE SAME COEFFICIENT MATRIX, WHICH IS SYMMETRIC, POSITIVE DEFINITE AND IN BANDFORM, PROVIDED THAT THIS MATRIX HAS BEEN DECOMPOSED BY A CALL OF THE PROCEDURE CHLDECBND (SECTION 3.1.2.1.1.2.1.1.).

B) CHLDECSOLBND, FOR THE SOLUTION OF ONE SYSTEM OF LINEAR EQUATIONS BY CHOLESKY'S SQUARE ROOT METHOD, PROVIDED THAT THE SYMMETRIC POSITIVE DEFINITE COEFFICIENT MATRIX IS IN BAND FORM AND IS STORED COLUMNWISE IN A ONE-DIMENSIONAL ARRAY.

KEYWORDS :

LINEAR EQUATIONS,  
CHOLESKY DECOMPOSITION,  
SYMMETRIC POSITIVE DEFINITE MATRIX,  
BAND MATRIX.

SUBSECTION : CHLSOLBND.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"PROCEDURE" CHLSOLBND(A, N, W, B); "VALUE" N, W; "INTEGER" N, W;  
"ARRAY" A, B;

THE MEANING OF THE FORMAL PARAMETERS IS :

A, N, W : SEE CALLING SEQUENCE OF CHLDECBND,  
THE CONTENTS OF THE ARRAY A ARE AS PRODUCED BY  
CHLDECBND;

B : <ARRAY IDENTIFIER>;  
"ARRAY" B[1 : N];

ENTRY : THE RIGHT HAND SIDE OF THE SYSTEM OF LINEAR  
EQUATIONS;

EXIT : THE SOLUTION OF THE SYSTEM.

PROCEDURES USED :

VEGVEC = CP34010,  
SCAPRD1 = CP34017.



## RUNNING TIME :

(C3 \* W + C4) \* N;  
 THE CONSTANTS C3 AND C4 DEPEND UPON THE  
 ARITHMETIC OF THE COMPUTER.

LANGUAGE : ALGOL 60.

## METHOD AND PERFORMANCE :

THE PROCEDURE CHLSOLBND CALCULATES THE SOLUTION OF A SYSTEM OF LINEAR EQUATIONS, PROVIDED THAT THE COEFFICIENT MATRIX WAS DECOMPOSED BY A SUCCESSFUL CALL OF CHLDECBND (SECTION 3.1.2.1.1.2.1.1.).

THE SOLUTION OF THE LINEAR SYSTEM IS OBTAINED BY CARRYING OUT THE FORWARD AND BACK SUBSTITUTION WITH THE CHOLESKY MATRIX AND THE RIGHT HAND SIDE. THE LATTER IS OVERWRITTEN BY THE SOLUTION. THE SOLUTIONS OF SEVERAL SYSTEMS WITH THE SAME COEFFICIENT MATRIX CAN BE OBTAINED BY SUCCESSIVE CALLS OF CHLSOLBND.

## EXAMPLE OF USE :

THE FOLLOWING PROGRAM SOLVES THE SYSTEM OF SIMULTANEOUS EQUATIONS

$$\begin{array}{rcl}
 2 * X1 & - & X2 & & & = & 1 \\
 - X1 & + & 2 * X2 & - & X3 & & = & 0 \\
 & & - X2 & + & 2 * X3 & - & X4 & = & 0 \\
 & & & & - X3 & + & 2 * X4 & - & X5 & = & 0 \\
 & & & & & & - X4 & + & 2 * X5 & = & 1
 \end{array}$$

```

"BEGIN""COMMENT" 730829, TEST CHLDECBND, CHLSOLBND AND
  CHLDETERMBND;
  "PROCEDURE" CHLDECBND(A, N, W, AUX); "CODE" 34330;
  "PROCEDURE" CHLSOLBND(A, N, W, B); "CODE" 34332;
  "REAL""PROCEDURE" CHLDETERMBND(A, N, W); "CODE" 34331;
  "INTEGER" I;
  "ARRAY" SYMBAND[1 : 9], RIGHT[1 : 5], AUX[2 : 3];
  "FOR" I:= 1 "STEP" 1 "UNTIL" 9 "DO"
  SYMBAND[I]:= "IF" I // 2 * 2 < I "THEN" 2 "ELSE" - 1;
  RIGHT[1]:= RIGHT[5]:= 1;
  "FOR" I:= 2, 3, 4 "DO" RIGHT[I]:= 0; AUX[2]:= "- 12;
  CHLDECBND(SYMBAND, 5, 1, AUX);
  "IF" AUX[3] = 5 "THEN"
  "BEGIN" CHLSOLBND(SYMBAND, 5, 1, RIGHT);
    OUTPUT(61, "("5(+2Z.4D2B), / "("DETERMINANT IS ") +.8D"+DD
    ")", (RIGHT[I], I:= 1 : 5), CHLDETERMBND(SYMBAND, 5, 1))
  "END"
"END".

```

THIS PROGRAM DELIVERS:

+1.0000 +1.0000 +1.0000 +1.0000 +1.0000  
 DETERMINANT IS +.60000000"+01

SUBSECTION: DECSOLSYMTRI.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" DECSOLSYMTRI(DIAG, CO, N, AUX, B);  
 "VALUE" N; "INTEGER" N; "ARRAY" DIAG, CO, AUX, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

DIAG: <ARRAY IDENTIFIER>;  
 "ARRAY" DIAG[1:N];  
 ENTRY: THE DIAGONAL OF THE GIVEN MATRIX T, SAY;  
 EXIT: SUPPOSE U DENOTES THE UNIT UPPER-BIDIAGONAL MATRIX,  
 SUCH THAT  $U'DU = T$  FOR SOME DIAGONAL MATRIX D,  
 WHERE U' DENOTES THE TRANSPOSED MATRIX; THEN D[I,I]  
 WILL BE DELIVERED IN DIAG[I], I = 1, ..., AUX[3];

CO: <ARRAY IDENTIFIER>;  
 "ARRAY" CO[1:N - 1];  
 ENTRY: THE CODIAGONAL OF T; T[I, I + 1] SHOULD BE GIVEN IN  
 CO[I], I = 1, ..., N - 1;  
 EXIT: U[I, I + 1] WILL BE DELIVERED IN CO[I], I = 1, ...,  
 AUX[3] - 1;

N: <ARITHMETICAL EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[2:5];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS, HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 EXIT:  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED;  
 AUX[5]: IF AUX[3] = N, THEN AUX[5] WILL EQUAL THE INFINITY-  
 NORM OF THE MATRIX, ELSE AUX[5] IS SET EQUAL TO  
 THE VALUE OF THAT ELEMENT WHICH CAUSES THE  
 BREAKDOWN OF THE DECOMPOSITION;

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: IF AUX[3] = N THEN THE SOLUTION OF THE LINEAR  
 SYSTEM IS OVERWRITTEN ON B, ELSE B REMAINS  
 UNALTERED.

## PROCEDURES USED:

DECSYMTRI = CP34420,  
SOLSYMTRI = CP34421.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

DECSOLSYMTRI CALCULATES THE SOLUTION OF A LINEAR SYSTEM WITH A SYMMETRIC TRIDIAGONAL MATRIX; THE TRIANGULAR DECOMPOSITION IS DONE BY CALLING DECSYMTRI (SECTION 3.1.2.1.1.2.2.1) AND THE FORWARD AND BACK SUBSTITUTION BY CALLING SOLSYMTRI (THIS SECTION); IF AUX[3]<N, THEN THE EFFECT OF DECSOLSYMTRI IS MERELY THAT OF DECSYMTRI.

## EXAMPLE OF USE:

LET T BE A SYMMETRIC TRIDIAGONAL MATRIX OF ORDER 100 WITH DIAGONAL ELEMENTS I (I = 1, ..., 100) AND CODIAGONAL ELEMENTS I \* 2 (I = 1, ..., 99); LET THE RIGHT HAND SIDE B BE GIVEN BY THE SECOND COLUMN OF T; THEN THE SOLUTION OF THE LINEAR SYSTEM TX = B IS GIVEN BY THE SECOND UNIT VECTOR; BY THE FOLLOWING PROGRAM WE MAY SOLVE THIS SYSTEM AND PRINT THE ERROR IN THE CALCULATED SOLUTION.

```

"BEGIN"
  "PROCEDURE" DECSOLSYMTRI(D, C, N, A, B); "CODE" 34422;
  "REAL" "PROCEDURE" VECVEC(L, U, S, A, B); "CODE" 34010;
  "INTEGER" I; "ARRAY" D, CO, B[1:100], AUX[2:5];
  "FOR" I:= 1 "STEP" 1 "UNTIL" 100 "DO"
  "BEGIN" D[I]:= I; CO[I]:= I * 2; B[I]:= 0 "END";
  B[1]:= B[2]:= 2; B[3]:= 4;
  AUX[2]:= "-14;
  DECSOLSYMTRI(D, CO, 100, AUX, B);
  B[2]:= B[2] - 1;
  OUTPUT(71, "(""/,"("      AUX[3] AND AUX[5]:")",2(/48,N)""",
  AUX[3], AUX[5]);
  OUTPUT(71, "(""/,"("      ERROR IN THE SOLUTION:")",N,/"")",
  SQR(VECVEC(1, 100, 0, B, B)))
"END"

```

## RESULTS:

```

AUX[3] AND AUX[5]:
+1.0000000000000000"+002
+4.9300000000000000"+002

```

```

ERROR IN THE SOLUTION:+0.0000000000000000"+000

```

AUTHOR: W. HOFFMANN,

CONTRIBUTOR: J. C. P. BUS,

INSTITUTE: MATHEMATICAL CENTRE,

RECEIVED: 731215.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS A PROCEDURE, DECSYMTRI, TO PERFORM A TRIANGULAR DECOMPOSITION OF A SYMMETRIC TRIDIAGONAL MATRIX.

KEYWORDS:

LU DECOMPOSITION,  
 TRIANGULAR DECOMPOSITION,  
 SYMMETRIC TRIDIAGONAL MATRIX.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:

"PROCEDURE" DECSYMTRI(DIAG, CO, N, AUX);  
 "VALUE" N; "INTEGER" N; "ARRAY" DIAG, CO, AUX;

THE MEANING OF THE FORMAL PARAMETERS IS:

DIAG: <ARRAY IDENTIFIER>;

"ARRAY" DIAG[1: N];

ENTRY: THE DIAGONAL OF THE GIVEN MATRIX T, SAY;

EXIT: SUPPOSE U DENOTES THE UNIT UPPER-BIDIAGONAL MATRIX,  
 SUCH THAT  $U'DU = T$  FOR SOME DIAGONAL MATRIX D,  
 WHERE  $U'$  DENOTES THE TRANSPOSED MATRIX; THEN  $D[I, I]$   
 WILL BE DELIVERED IN  $DIAG[I]$ ,  $I = 1, \dots, AUX[3]$ ;

CO: <ARRAY IDENTIFIER>;

"ARRAY" CO[1: N - 1];

ENTRY: THE CODIAGONAL OF T;  $T[I, I + 1]$  SHOULD BE GIVEN IN  
 $CO[I]$ ,  $I = 1, \dots, N - 1$ ;

EXIT:  $U[I, I + 1]$  WILL BE DELIVERED IN  $CO[I]$ ,  $I = 1, \dots,$   
 $AUX[3] - 1$ ;

N: <ARITHMETICAL EXPRESSION>;

THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;

"ARRAY" AUX[2:5];

ENTRY:

AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS, HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;

EXIT:

AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED;

AUX[5]: IF  $AUX[3] = N$ , THEN  $AUX[5]$  WILL EQUAL THE INFINITY-  
 NORM OF THE MATRIX, ELSE  $AUX[5]$  IS SET EQUAL TO  
 THE VALUE OF THAT ELEMENT WHICH CAUSES THE  
 BREAKDOWN OF THE DECOMPOSITION.

PROCEDURES USED: NONE.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE METHOD USED IN DECSYMTRI YIELDS A UNIT UPPER-BIDIAGONAL MATRIX U AND A DIAGONAL MATRIX D, SUCH THAT THE PRODUCT U'DU EQUALS THE GIVEN SYMMETRIC TRIDIAGONAL MATRIX; THE PROCESS IS TERMINATED IN THE K-TH STEP IF THE MODULUS OF THE K-TH DIAGONAL ELEMENT IS SMALLER THAN A CERTAIN SMALL VALUE, WHICH IS GIVEN BY AUX[2] MULTIPLIED BY THE 1-NORM OF THE K-TH ROW; IN THIS CASE AUX[3] WILL BE GIVEN THE VALUE  $K - 1$  AND AUX[5] WILL BE GIVEN THE VALUE OF THE K-TH DIAGONAL ELEMENT.

EXAMPLE OF USE: SEE DECSOLSYMTRI (SECTION 3.1.2.1.1.2.2.3).

SOURCE TEXT:

```
"CODE" 34420;
"PROCEDURE" DECSYMTRI(DIAG, CO, N, AUX); "VALUE" N; "INTEGER" N;
"ARRAY" DIAG, CO, AUX;
"BEGIN" "INTEGER" I, N1;
"REAL" D, R, S, U, TOL, NORM, NORMR;
TOL:= AUX[2]; D:= DIAG[1]; R:= CO[1];
NORM:= NORMR:= ABS(D) + ABS(R);
"IF" ABS(D) <= NORMR * TOL "THEN"
"BEGIN" AUX[3]:= 0; AUX[5]:= D; "GOTO" EXIT "END";
U:= CO[1]:= R / D; N1:= N - 1;
"FOR" I:= 2 "STEP" 1 "UNTIL" N1 "DO"
"BEGIN" S:= R; R:= CO[I]; D:= DIAG[I];
NORMR:= ABS(S) + ABS(D) + ABS(R);
D:= DIAG[I]:= D - U * S;
"IF" ABS(D) <= NORMR * TOL "THEN"
"BEGIN" AUX[3]:= I - 1; AUX[5]:= D; "GOTO" EXIT "END";
U:= CO[I]:= R / D; "IF" NORMR > NORM "THEN" NORM:= NORMR
"END";
D:= DIAG[N]; NORMR:= ABS(D) + ABS(R);
D:= DIAG[N]:= D - U * R;
"IF" ABS(D) <= NORMR * TOL "THEN"
"BEGIN" AUX[3]:= N1; AUX[5]:= D; "GOTO" EXIT "END";
"IF" NORMR > NORM "THEN" NORM:= NORMR;
AUX[3]:= N; AUX[5]:= NORM;
EXIT;
"END" DECSYMTRI;
"EOB"
```

SECTION 3.1.2.1.1.2.2.3

(JUNE 1974)

PAGE 1

AUTHOR: W. HOFFMANN.

CONTRIBUTOR: J. C. P. BUS.

INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED: 731215.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS TWO PROCEDURES FOR SOLVING A SYSTEM OF LINEAR EQUATIONS WITH A SYMMETRIC TRIDIAGONAL MATRIX; SOLSYMTRI CALCULATES A SOLUTION IF THE SOLSYMTRI CALCULATES A SOLUTION IF THE TRIANGULARLY DECOMPOSED FORM, AS DELIVERED BY DECSYMTRI (SECTION 3.1.2.1.1.2.2.1), IS GIVEN; DECSOLSYMTRI PERFORMS THE TRIANGULAR DECSOLSYMTRI PERFORMS THE TRIANGULAR DECOMPOSITION AS WELL AS THE FORWARD AND BACK SUBSTITUTION TO CALCULATE THE SOLUTION OF THE GIVEN LINEAR SYSTEM.

KEYWORDS:

ALGEBRAIC EQUATIONS,  
 LINEAR SYSTEMS,  
 SYMMETRIC TRIDIAGONAL MATRIX,  
 FORWARD AND BACK SUBSTITUTION.

SUBSECTION: SOLSYMTRI.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" SOLSYMTRI(DIAG, CO, N, B);  
 "VALUE" N; "INTEGER" N; "ARRAY" DIAG, CO, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

DIAG: <ARRAY IDENTIFIER>;  
 "ARRAY" DIAG[1:N];  
 ENTRY: THE DIAGONAL MATRIX, AS  
 DELIVERED BY DECSYMTRI (SECTION 3.1.2.1.1.2.2.1);  
 CO: <ARRAY IDENTIFIER>;  
 "ARRAY" CO[1: N - 1];  
 ENTRY: THE CODIAGONAL OF THE UNIT  
 UPPER-BIDIAGONAL MATRIX AS DELIVERED BY DECSYMTRI;  
 N: <ARITHMETICAL EXPRESSION>;  
 THE ORDER OF THE MATRIX;  
 B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: THE CALCULATED SOLUTION OF THE LINEAR SYSTEM.

PROCEDURES USED: NONE.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SOLSYMTRI CALCULATES THE SOLUTION OF A LINEAR SYSTEM WITH A SYMMETRIC TRIDIAGONAL MATRIX, WITH FORWARD AND BACK SUBSTITUTION; THE TRIANGULARLY DECOMPOSED FORM OF THE MATRIX, AS PRODUCED BY DECSYMTRI (SECTION 3.1.2.1.1.2.2.1), SHOULD BE GIVEN; ONE CALL OF DECSYMTRI FOLLOWED BY SEVERAL CALLS OF SOLSYMTRI MAY BE USED TO SOLVE SEVERAL LINEAR SYSTEMS HAVING THE SAME SYMMETRIC TRIDIAGONAL MATRIX, BUT DIFFERENT RIGHT HAND SIDES.

EXAMPLE OF USE: SEE DECSOLSYMTRI (THIS SECTION).

## SUBSECTION: DECSOLSYMTRI.

## CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS;  
 "PROCEDURE" DECSOLSYMTRI(DIAG, CO, N, AUX, B);  
 "VALUE" N; "INTEGER" N; "ARRAY" DIAG, CO, AUX, B;

## THE MEANING OF THE FORMAL PARAMETERS IS:

DIAG: <ARRAY IDENTIFIER>;  
 "ARRAY" DIAG[1:N];  
 ENTRY: THE DIAGONAL OF THE GIVEN MATRIX T, SAY;  
 EXIT: SUPPOSE U DENOTES THE UNIT UPPER-BIDIAGONAL MATRIX,  
 SUCH THAT  $U'UD = T$  FOR SOME DIAGONAL MATRIX D,  
 WHERE U' DENOTES THE TRANSPOSED MATRIX; THEN D[I,I]  
 WILL BE DELIVERED IN DIAG[I], I = 1, ..., AUX[3];

CO: <ARRAY IDENTIFIER>;  
 "ARRAY" CO[1:N-1];  
 ENTRY: THE CODIAGONAL OF T; T[I, I+1] SHOULD BE GIVEN IN  
 CO[I], I = 1, ..., N-1;  
 EXIT: U[I, I+1] WILL BE DELIVERED IN CO[I], I = 1, ...,  
 AUX[3] - 1;

N: <ARITHMETICAL EXPRESSION>;  
 THE ORDER OF THE MATRIX;

AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX[2:5];  
 ENTRY:  
 AUX[2]: A RELATIVE TOLERANCE; A REASONABLE CHOICE FOR THIS  
 VALUE IS AN ESTIMATE OF THE RELATIVE PRECISION OF  
 THE MATRIX ELEMENTS, HOWEVER, IT SHOULD NOT BE  
 CHOSEN SMALLER THAN THE MACHINE PRECISION;  
 EXIT:  
 AUX[3]: THE NUMBER OF ELIMINATION STEPS PERFORMED;  
 AUX[5]: IF AUX[3] = N, THEN AUX[5] WILL EQUAL THE INFINITY-  
 NORM OF THE MATRIX, ELSE AUX[5] IS SET EQUAL TO  
 THE VALUE OF THAT ELEMENT WHICH CAUSES THE  
 BREAKDOWN OF THE DECOMPOSITION;

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 ENTRY: THE RIGHT HAND SIDE OF THE LINEAR SYSTEM;  
 EXIT: IF AUX[3] = N THEN THE SOLUTION OF THE LINEAR  
 SYSTEM IS OVERWRITTEN ON B, ELSE B REMAINS  
 UNALTERED.



## PROCEDURES USED:

```

DECSYMTRI = CP34420,
SOLSYMTRI = CP34421,
    
```

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

DECSOLSYMTRI CALCULATES THE SOLUTION OF A LINEAR SYSTEM WITH A SYMMETRIC TRIDIAGONAL MATRIX; THE TRIANGULAR DECOMPOSITION IS DONE BY CALLING DECSYMTRI (SECTION 3.1.2.1.1.2.2.1) AND THE FORWARD AND BACK SUBSTITUTION BY CALLING SOLSYMTRI (THIS SECTION); IF AUX[3]=N, THEN THE EFFECT OF DECSOLSYMTRI IS MERELY THAT OF DECSYMTRI.

## EXAMPLE OF USE:

LET T BE A SYMMETRIC TRIDIAGONAL MATRIX OF ORDER 100 WITH DIAGONAL ELEMENTS I (I = 1, ..., 100) AND CODIAGONAL ELEMENTS I \* 2 (I = 1, ..., 99); LET THE RIGHT HAND SIDE B BE GIVEN BY THE SECOND COLUMN OF T; THEN THE SOLUTION OF THE LINEAR SYSTEM TX = B IS GIVEN BY THE SECOND UNIT VECTOR; BY THE FOLLOWING PROGRAM WE MAY SOLVE THIS SYSTEM AND PRINT THE ERROR IN THE CALCULATED SOLUTION.

```

"BEGIN"
  "PROCEDURE" DECSOLSYMTRI(D, C, N, A, B); "CODE" 34422;
  "REAL" "PROCEDURE" VECVEC(L, U, S, A, B); "CODE" 34010;
  "INTEGER" I; "ARRAY" D, CO, B[1:100], AUX[2:5];
  "FOR" I:= 1 "STEP" 1 "UNTIL" 100 "DO"
    "BEGIN" D[I]:= I; CO[I]:= I * 2; B[I]:= 0 "END";
  B[1]:= B[2]:= 2; B[3]:= 4;
  AUX[2]:= "-14;
  DECSOLSYMTRI(D, CO, 100, AUX, B);
  B[2]:= B[2] - 1;
  OUTPUT(71, "(//, "("      AUX[3] AND AUX[5]:"), 2(/4B, N)");
  AUX[3], AUX[5]);
  OUTPUT(71, "(//, "("      ERROR IN THE SOLUTION:"), N, /");
  SQRT(VECVEC(1, 100, 0, B, B))
"END"
    
```

## RESULTS:

```

AUX[3] AND AUX[5]:
+1,0000000000000000"+002
+4,9300000000000000"+002
    
```

```

ERROR IN THE SOLUTION:+0,0000000000000000"+000
    
```

## SOURCE TEXTS:

```

"CODE" 34421;
"PROCEDURE" SOLSYMTRI(DIAG, CO, N, B); "VALUE" N; "INTEGER" N;
"ARRAY" DIAG, CO, B;
"BEGIN" "INTEGER" I;
  "REAL" R, S;
  R:= B[1]; B[1]:= R / DIAG[1];
  "FOR" I:= 2 "STEP" 1 "UNTIL" N "DO"
    "BEGIN" R:= B[I] - CO[I-1] * R; B[I]:= R / DIAG[I] "END";
  S:= B[N];
  "FOR" I:= N - 1 "STEP" -1 "UNTIL" 1 "DO"
    S:= B[I]:= B[I] - CO[I] * S
"END" SOLSYMTRI;
"EOB"

```

```

"CODE" 34422;
"PROCEDURE" DECSOLSYMTRI(DIAG, CO, N, AUX, B); "VALUE" N;
"INTEGER" N; "ARRAY" DIAG, CO, AUX, B;
"BEGIN" "PROCEDURE" DECSYMTRI(DIAG, CO, N, AUX); "CODE" 34420;
  "PROCEDURE" SOLSYMTRI(DIAG, CO, N, B); "CODE" 34421;
  DECSYMTRI(DIAG, CO, N, AUX); "IF" AUX[3] = N "THEN"
    SOLSYMTRI(DIAG, CO, N, B)
"END" DECSOLSYMTRI;
"EOB"

```

AUTHOR: P.W.HEMKER.

INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED: 730615.

## BRIEF DESCRIPTION:

CONJ GRAD SOLVES A LINEAR SYSTEM OF EQUATIONS BY THE METHOD OF CONJUGATE GRADIENTS. THE SYSTEM HAS TO BE SYMMETRIC AND POSITIVE DEFINITE.

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:

"PROCEDURE" CONJ GRAD (MATVEC, X, R, L, N, GO ON, ITERATE, NORM2);  
 "VALUE" L, N; "BOOLEAN" GO ON; "INTEGER" L, N, ITERATE;  
 "REAL" NORM2; "ARRAY" X, R; "PROCEDURE" MATVEC;

THE MEANING OF THE FORMAL PARAMETERS IS:

MATVEC: <PROCEDURE IDENTIFIER>;

THE HEADING OF THIS PROCEDURE READS:

"PROCEDURE" MATVEC( P, Q); "ARRAY" P, Q;

THIS PROCEDURE DEFINES THE MATRIX A (THE COEFFICIENT MATRIX OF THE SYSTEM) AS FOLLOWS :

AT EACH CALL MATVEC DELIVERS IN Q THE MATRIX-VECTOR PRODUCT AP; P AND Q ARE ONE - DIMENSIONAL ARRAYS:

"ARRAY" P,Q[L:N];

X: <ARRAY IDENTIFIER>;

"ARRAY" X[L:N];

ENTRY: AN INITIAL APPROXIMATION TO THE SOLUTION X;

EXIT: THE SOLUTION;

R: <ARRAY IDENTIFIER>;

"ARRAY" R[L:N];

ENTRY: THE RIGHT-HAND SIDE OF THE SYSTEM;

EXIT: THE RESIDUE B - AX, COMPUTED RECURSIVELY;

L,N: <ARITHMETIC EXPRESSION>;

L AND N ARE RESPECTIVELY THE LOWER AND UPPER BOUND OF THE ARRAYS X,R,P,Q;

GO ON: <BOOLEAN EXPRESSION>;

GO ON INDICATES THE CONTINUATION OF THE PROCESS.

THIS EXPRESSION MAY DEPEND ON THE JENSEN PARAMETERS ITERATE AND NORM2. WITH THIS BOOLEAN EXPRESSION THE USER CONTROLS THE CONTINUATION OF THE PROCESS. IF GO ON:= "FALSE" THE ITERATION PROCESS IS STOPPED.

ITERATE: <IDENTIFIER>;

DELIVERS THE NUMBER OF ITERATION STEPS ALREADY PERFORMED;

NORM2: <IDENTIFIER>;

DELIVERS THE SQUARED EUCLIDIC NORM OF THE RESIDUE, COMPUTED RECURSIVELY

PROCEDURES USED:

VECVEC = CP34010 ,  
ELMVEC = CP34020 .

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:  $7 + 2 * ( N - L + 1 )$ .

RUNNING TIME:

THE RUNNING TIME IS PROPORTIONAL TO THE NUMBER OF ITERATION STEPS PERFORMED. EACH ITERATION STEP REQUIRES ONE EVALUATION OF THE PROCEDURE MATVEC, THE EVALUATION OF TWO SCALAR - VECTOR - PRODUCTS AND ONE VECTOR - VECTOR - PRODUCT.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE REF[1].

REFERENCES:

- [1]. J.K.REID.  
ON THE METHOD OF CONJUGATE GRADIENTS FOR THE SOLUTION OF LARGE SPARSE SYSTEMS OF LINEAR EQUATIONS.  
IN: LARGE SPARSE SETS OF LINEAR EQUATIONS (J.K.REID ED) 1971.

EXAMPLE OF USE:

```

"BEGIN"
  "PROCEDURE" CONJ GRAD(A,X,R,L,N,GO ON,IT,NO);"CODE" 34220;
  "ARRAY" X,B[0:12];
  "INTEGER" IT,I;
  "REAL" NO;
  "PROCEDURE" A(X,B);
  "ARRAY" X,B;
  "BEGIN" B[0]:=2*X[0]-X[1];
    "FOR" I:=1 "STEP" 1 "UNTIL" 11 "DO"
      B[I]:=-X[I-1]+2*X[I]-X[I+1];
      B[12]:=2*X[12]-X[11]
  "END" A;
  "FOR" I:=0 "STEP" 1 "UNTIL" 12 "DO" X[I]:=B[I]:=0;
  B[0]:=1;B[12]:=4;
  CONJ GRAD(A,X,B,0,12,IT<20 "AND" NO>"=10,IT,NO);
  OUTPUT(61,"("IT="),B3D5B,("NO="),N,/,/,10B,
    ("X"),20B,("R"),/,/),IT,NO);
  "FOR" I:=0 "STEP" 1 "UNTIL" 12 "DO"
  OUTPUT(61,("N,5B,N"),X[I],B[I])
"END"

```

DELIVERS:

IT= 013      NO= +3,3424581859911"-027

X

R

+1,2142857142857"+000	=7,1054273576010"-015
+1,4285714285715"+000	+1,5151278924296"-014
+1,6428571428572"+000	-1,3184703260130"-014
+1,8571428571429"+000	+1,6718441615946"-014
+2,0714285714286"+000	-1,5514524667596"-014
+2,2857142857144"+000	+2,2130179956186"-014
+2,5000000000001"+000	-2,2524167805437"-014
+2,7142857142858"+000	+2,0834049529361"-014
+2,9285714285715"+000	-1,8674557504802"-014
+3,1428571428572"+000	+1,9163204503355"-014
+3,3571428571429"+000	-1,2366043539824"-014
+3,5714285714286"+000	+8,2548347242718"-015
+3,7857142857143"+000	+4,4408920985006"-016

SOURCE TEXT(S):

```

"CODE" 34220;
"PROCEDURE" CONJ GRAD( MATVEC, X, R, L, N, GO ON, ITERATE, NORM2);
"VALUE" L, N; "PROCEDURE" MATVEC; "ARRAY" X, R; "BOOLEAN" GO ON;
"INTEGER" L, N, ITERATE; "REAL" NORM2;
"BEGIN" "ARRAY" P, AP[ L: N];
  "INTEGER" I;
  "REAL" A, B, PRR, RRP;
  "REAL" "PROCEDURE" VECVEC( A, B, C, D, E); "CODE" 34010;
  "PROCEDURE" ELMVEC( A, B, C, D, E, F); "CODE" 34020;
  "FOR" ITERATE:= 0, ITERATE + 1 "WHILE" GO ON "DO"
  "BEGIN" "IF" ITERATE = 0 "THEN"
    "BEGIN" MATVEC( X, P);
      "FOR" I:= L "STEP" 1 "UNTIL" N "DO"
        P[ I]:= R[ I]:= R[ I] - P[ I];
        PRR:= VECVEC( L, N, 0, R, R)
      "END" "ELSE"
        "BEGIN" B:= RRP / PRR; PRR:= RRP;
          "FOR" I:= L "STEP" 1 "UNTIL" N "DO"
            P[ I]:= R[ I] + B * P[ I]
          "END";
        MATVEC( P, AP);
        A:= PRR / VECVEC( L, N, 0, P, AP);
        ELMVEC( L, N, 0, X, P, A);
        ELMVEC( L, N, 0, R, AP, -A);
        NORM2:= RRP:= VECVEC( L, N, 0, R, R)
    "END"
  "END" CONJ GRAD;
"EOP"

```

SECTION: 3, 2, 1, 1, 1

(JUNE 1974)

PAGE 1

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CONTRIBUTORS: W, HOFFMANN, J, G, VERWER.

INSTITUTE: MATHEMATICAL CENTRE.

RECEIVED: 731022.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS TWO PROCEDURES.  
 A) EQILBR EQUILIBRATES A MATRIX BY MEANS OF A DIAGONAL SIMILARITY TRANSFORMATION,  
 B) BAKLBR PERFORMS THE CORRESPONDING BACK TRANSFORMATION ON THE COLUMNS OF A MATRIX AND SHOULD BE CALLED AFTER EQILBR.

KEYWORDS:

SIMILARITY TRANSFORMATION,  
 EQUILIBRATION.

SUBSECTION: EQILBR.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" EQILBR(A, N, EM, D, INT); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, EM, D; "INTEGER" "ARRAY" INT;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE MATRIX TO BE EQUILIBRATED;  
 EXIT: THE EQUILIBRATED MATRIX;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:0];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 D: <ARRAY IDENTIFIER>;  
 "ARRAY" D[1:N];  
 EXIT: THE MAIN DIAGONAL OF THE TRANSFORMING DIAGONAL MATRIX;  
 INT: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" INT[1:N];  
 EXIT: INFORMATION DEFINING THE POSSIBLE INTERCHANGING OF SOME ROWS AND THE CORRESPONDING COLUMNS;

SECTION:3,2,1,1.1

(JUNE 1974)

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PROCEDURES USED:

TAMMAT	=	CP34014,
MATTAM	=	CP34015,
ICHCOL	=	CP34031,
ICHROW	=	CP34032.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N SQUARED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE MATRIX IS EQUILIBRATED BY MEANS OF OSBORNE'S DIAGONAL SIMILARITY TRANSFORMATION POSSIBLY WITH INTERCHANGES [2]. THE TRANSFORMING DIAGONAL MATRIX AND THE EQUILIBRATED MATRIX ARE CALCULATED ITERATIVELY:

IN EACH STEP A CERTAIN COLUMN OF THE MATRIX IS MULTIPLIED BY, AND THE CORRESPONDING ROW DIVIDED BY, A FACTOR WHICH IS CHOSEN IN SUCH A WAY THAT THE CONSIDERED COLUMN AND ROW OBTAIN ROUGHLY THE SAME EUCLIDEAN NORM (IN FACT, THE FACTOR IS ROUNDED TO THE NEAREST INTEGRAL POWER OF 2, IN ORDER TO PREVENT ROUNDING ERRORS); THE COLUMNS AND ROWS ARE HANDLED IN CYCLIC ORDER, IF THE MATRIX DOES NOT CONTAIN COLUMNS OR ROWS WHOSE OFF-DIAGONAL ELEMENTS ARE 0 OR NEARLY 0, THEN THE PROCESS (WITH UNROUNDED FACTORS) CONVERGES, AND IN PRACTICE A FEW STEPS ARE NEEDED TO OBTAIN A REASONABLY EQUILIBRATED MATRIX [2].

IF ALL OFF-DIAGONAL ELEMENTS OF SOME CONSIDERED COLUMN (ROW) ARE 0 OR NEARLY 0, THEN THIS COLUMN (ROW) IS INTERCHANGED WITH THE FIRST NONZERO COLUMN (LAST NONZERO ROW) OF THE MATRIX, AND, IN ORDER TO HAVE A SIMILARITY TRANSFORMATION, THE CORRESPONDING ROWS (COLUMNS) ARE ALSO INTERCHANGED; THEN FOR THE FURTHER EQUILIBRATION, THE SUBMATRIX IS CONSIDERED WHICH DOES NOT CONTAIN SUCH ZERO COLUMNS AND ROWS AND THE CORRESPONDING ROWS AND COLUMNS. THE EQUILIBRATION PROCESS IS CONTINUED UNTIL, IN A WHOLE CYCLE NO FACTOR  $> 2$  OR  $< 0.5$  AND NO ZERO COLUMN OR ROW IS FOUND, OR UNTIL  $(N + 1) * N ** 2$  ROWS AND COLUMNS HAVE BEEN CONSIDERED.



SUBSECTION: BAKLBR.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" BAKLBR(N, N1, N2, D, INT, VEC); "VALUE" N, N1, N2;  
 "INTEGER" N, N1, N2; "ARRAY" D, VEC; "INTEGER" "ARRAY" INT;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE LENGTH OF THE VECTORS TO BE TRANSFORMED;  
 N1, N2: <ARITHMETIC EXPRESSION>;  
 THE SERIAL NUMBERS OF THE FIRST AND LAST VECTOR TO BE  
 TRANSFORMED;  
 VEC: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC [1:N, N1:N2];  
 ENTRY: THE  $N2 - N1 + 1$  VECTORS OF LENGTH N TO BE  
 TRANSFORMED;  
 EXIT: THE  $N2 - N1 + 1$  VECTORS OF LENGTH N RESULTING FROM  
 THE BACK TRANSFORMATION;  
 D: <ARRAY IDENTIFIER>;  
 "ARRAY" D [1:N];  
 ENTRY: THE MAIN DIAGONAL OF THE TRANSFORMING DIAGONAL  
 MATRIX OF ORDER N, AS PRODUCED BY EQILBR;  
 INT: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" INT [1:N];  
 ENTRY: INFORMATION DEFINING THE POSSIBLE INTERCHANGING OF  
 SOME ROWS AND COLUMNS, AS PRODUCED BY EQILBR.

PROCEDURES USED:

ICHROW                    ■            CP34032.

RUNNING TIME: ROUGHLY PROPORTIONAL TO  $(N2 - N1 + 1) * N$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE BACK TRANSFORMATION, WHICH CORRESPONDS WITH THE DIAGONAL  
 SIMILARITY TRANSFORMATION AS PERFORMED BY EQILBR, TRANSFORMS  
 A VECTOR X INTO A VECTOR DX AND PERFORMS THE CORRESPONDING  
 INTERCHANGES. THE MATRIX D IS THE DIAGONAL MATRIX OF THE DIAGONAL  
 SIMILARITY TRANSFORMATION.

REFERENCES:

- [1] DEKKER, T. J. AND HOFFMANN, W.  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2,  
 MATHEMATICAL CENTRE TRACTS 23,  
 MATHEMATISCH CENTRUM, AMSTERDAM, 1968;
- [2] OSBORNE, E. E., ON PRECONDITIONING OF MATRICES,  
 J. ACM 7(1960) 338-354.

EXAMPLES OF USE:

EXAMPLES OF USE OF EQILBR AND BAKLBR CAN BE FOUND IN THE PROCEDURES  
 FOR CALCULATING EIGENVALUES AND EIGENVECTORS AS DESCRIBED IN  
 SECTION 3,3,1,2,2.

## SOURCE TEXT(S) :

```

"CODE" 34173;
"COMMENT" MCA 2405;
"PROCEDURE" EQILBR(A, N, EM, D, INT); "VALUE" N; "INTEGER" N;
"ARRAY" A, EM, D; "INTEGER" "ARRAY" INT;
"BEGIN" "INTEGER" I, IM, I1, P, Q, J, T, COUNT, EXPONENT, NI;
"REAL" C, R, EPS, OMEGA, FACTOR;

"PROCEDURE" MOVE(K); "VALUE" K; "INTEGER" K;
"BEGIN" "REAL" DI;
  NI:= Q - P; T:= T + 1; "IF" K ^= I "THEN"
  "BEGIN" ICHCOL(1, N, K, I, A); ICHROW(1, N, K, I, A);
  DI:= D[I]; D[I]:= D[K]; D[K]:= DI
  "END"
"END" MOVE;

"REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B); "CODE" 34014;
"REAL" "PROCEDURE" MATTAM(L, U, I, J, A, B); "CODE" 34015;
"PROCEDURE" ICHCOL(L, U, I, J, A); "CODE" 34031;
"PROCEDURE" ICHROW(L, U, I, J, A); "CODE" 34032;

FACTOR:= 1 / (2 * LN(2)); "COMMENT" MORE GENERALLY: LN(BASE);
EPS:= EM[0]; OMEGA:= 1 / EPS; T:= P:= 1; Q:= NI:= I:= N;
COUNT:= (N + 1) * N // 2;
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" D[J]:= 1; INT[J]:= 0 "END";
"FOR" I:= "IF" I < Q "THEN" I + 1 "ELSE" P
"WHILE" COUNT > 0 "AND" NI > 0 "DO"
"BEGIN" COUNT:= COUNT - 1; IM:= I - 1; I1:= I + 1;
  C:= SQRT(TAMMAT(P, IM, I, I, A, A) +
  TAMMAT(I1, Q, I, I, A, A));
  R:= SQRT(MATTAM(P, IM, I, I, A, A) +
  MATTAM(I1, Q, I, I, A, A));
  "IF" C * OMEGA <= R * EPS "THEN"
  "BEGIN" INT[T]:= I; MOVE(P); P:= P + 1 "END"
  "ELSE" "IF" R * OMEGA <= C * EPS "THEN"
  "BEGIN" INT[T]:= -I; MOVE(Q); Q:= Q - 1 "END"
  "ELSE"
  "BEGIN" EXPONENT:= LN(R / C) * FACTOR;
  "IF" ABS(EXPONENT) > 1 "THEN"
  "BEGIN" NI:= Q - P; C:= 2 ** EXPONENT; R:= 1 / C;
  D[I]:= D[I] * C;
  "FOR" J:= 1 "STEP" 1 "UNTIL" IM,
  I1 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" A[J, I]:= A[J, I] * C;
  A[I, J]:= A[I, J] * R
  "END"
  "END" "ELSE" NI:= NI - 1
  "END"
"END"
"END" EQILBR;
"EOF"

```

```

"CODE" 34174;
"COMMENT" MCA 2406;
"PROCEDURE" BAKLBR(N, N1, N2, D, INT, VEC); "VALUE" N, N1, N2;
"INTEGER" N, N1, N2; "ARRAY" D, VEC; "INTEGER" "ARRAY" INT;
"BEGIN" "INTEGER" I, J, K, P, Q; "REAL" DI;

      "PROCEDURE" ICHROW(L, U, I, J, A); "CODE" 34032;

      P:= 1; Q:= N;
      "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" DI:= D[I]; "IF" DI # 1 "THEN"
        "FOR" J:= N1 "STEP" 1 "UNTIL" N2 "DO" VEC[I,J]:=
          VEC[I,J] * DI; K:= INT[I];
        "IF" K > 0 "THEN" P:= P + 1 "ELSE"
        "IF" K < 0 "THEN" Q:= Q - 1
      "END";
      "FOR" I:= P - 1 + N - Q "STEP" -1 "UNTIL" 1 "DO"
      "BEGIN" K:= INT[I]; "IF" K > 0 "THEN"
        "BEGIN" P:= P - 1; "IF" K # P "THEN"
          ICHROW(N1, N2, K, P, VEC)
        "END" "ELSE"
        "BEGIN" Q:= Q + 1; "IF" -K # Q "THEN"
          ICHROW(N1, N2, -K, Q, VEC)
        "END"
      "END"
"END"
"END" BAKLBR;
"EOP"

```

SECTION: 3,2,1,1,2

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PAGE 1

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BRIEF DESCRIPTION :

THIS SECTION CONTAINS THE PROCEDURES EQUILBRCOM AND BAKLBRCOM.  
 EQUILBRCOM EQUILIBRATES A GIVEN MATRIX.  
 BAKLBRCOM TRANSFORMS THE EIGENVECTORS OF THE EQUILIBRATED MATRIX  
 INTO THE EIGENVECTORS OF THE ORIGINAL MATRIX.

KEYWORDS :

COMPLEX MATRIX,  
 EIGENVECTORS,  
 EQUILIBRATION.

SUBSECTION: EQUILBRCOM,

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "PROCEDURE" EQUILBRCOM(A1, A2, N, EM, D, INT); "VALUE" N;  
 "INTEGER" N; "ARRAY" A1, A2, EM, D; "INTEGER" "ARRAY" INT;

THE MEANING OF THE FORMAL PARAMETERS IS:

A1, A2: <ARRAY IDENTIFIER>;  
 "ARRAY" A1, A2 [1:N, 1:N];  
 ENTRY:  
 THE REAL PART AND IMAGINARY PART OF THE MATRIX TO BE  
 EQUILIBRATED MUST BE GIVEN IN THE ARRAYS A1 AND A2,  
 RESPECTIVELY;  
 EXIT:  
 THE REAL PART AND THE IMAGINARY PART OF THE EQUILIBRATED  
 MATRIX ARE DELIVERED IN THE ARRAYS A1 AND A2,  
 RESPECTIVELY;  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM [0:7];  
 ENTRY:  
 EM[0]: THE MACHINE PRECISION;  
 EM[6]: THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 EXIT:  
 EM[7]: THE NUMBER OF ITERATIONS PERFORMED;

```

D:      <ARRAY IDENTIFIER>;
        "ARRAY" D[1:N];
        EXIT;
        THE SCALING FACTORS OF THE DIAGONAL SIMILARITY
        TRANSFORMATION;
INT:    <ARRAY IDENTIFIER>;
        "INTEGER" "ARRAY" INT[1:N];
        EXIT;
        INFORMATION CONCERNING THE POSSIBLE INTERCHANGING OF
        SOME ROWS AND CORRESPONDING COLUMNS.

```

PROCEDURES USED:

```

ICHCOL = CP34031,
ICHROW = CP34332,
TAMMAT = CP34014,
MATTAM = CP34015.

```

RUNNING TIME: PROPORTIONAL TO  $N \times$  NUMBER OF ITERATIONS.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE BAKLBRCOM.

SUBSECTION: BAKLBRCOM.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "PROCEDURE" BAKLBRCOM(N, N1, N2, D, INT, VR, VI);  
 "VALUE" N, N1, N2; "INTEGER" N, N1, N2; "ARRAY" D, VR, VI;  
 "INTEGER" "ARRAY" INT;

THE MEANING OF THE FORMAL PARAMETERS IS:

```

N:      <ARITHMETIC EXPRESSION>;
        THE ORDER OF THE MATRIX OF WHICH THE EIGENVECTORS ARE
        CALCULATED;
N1, N2: <ARITHMETIC EXPRESSION>;
        THE EIGENVECTORS CORRESPONDING TO THE EIGENVALUES WITH
        INDICES N1, ..., N2 ARE TO BE TRANSFORMED;
D:      <ARRAY IDENTIFIER>;
        "ARRAY" D[1:N];
        ENTRY: THE SCALING FACTORS OF THE DIAGONAL SIMILARITY
        TRANSFORMATION AS DELIVERED BY EQILBRCOM;
INT:    <ARRAY IDENTIFIER>;
        "INTEGER" "ARRAY" INT[1:N];
        ENTRY: INFORMATION DEFINING THE INTERCHANGING OF SOME
        ROWS AND COLUMNS, AS DELIVERED BY EQILBRCOM;

```

VR, VI: <ARRAY IDENTIFIER>;  
 "ARRAY" VR, VI[1:N, N1:N2];  
 ENTRY:  
 THE BACK TRANSFORMATION IS PERFORMED ON THE EIGENVECTORS  
 WITH THE REAL PARTS GIVEN IN ARRAY VR AND THE IMAGINARY  
 PARTS GIVEN IN ARRAY VI;  
 EXIT:  
 THE REAL PARTS AND IMAGINARY PARTS OF THE RESULTING  
 EIGENVECTORS ARE DELIVERED IN THE COLUMNS OF THE ARRAYS  
 VR AND VI, RESPECTIVELY.

PROCEDURES USED: BAKLBR = CP34174.

RUNNING TIME: ROUGHLY PROPORTIONAL TO  $N * (N2 - N1)$ .

LANGUAGE: ALGOL 60.

THE FOLLOWING HOLDS FOR BOTH PROCEDURES:

#### METHOD AND PERFORMANCE:

A MATRIX  $M$  IS SAID TO BE EQUILIBRATED, WHEN THE DIAGONAL ELEMENTS  
 OF  $M^*M - MM^*$  ARE ZERO, WHERE  $*$  STANDS FOR CONJUGATING  
 AND TRANSPOSING. IN EQILBRCOM THE MATRIX  $M$  IS EQUILIBRATED  
 BY MEANS OF OSBORNE'S DIAGONAL SIMILARITY TRANSFORMATION WITH  
 POSSIBLE INTERCHANGES (OSBORNE, 1960).  
 BAKLBRCOM PERFORMS THE CORRESPONDING BACK TRANSFORMATION.  
 LET THE EIGENVECTORS OF THE EQUILIBRATED MATRIX BE GIVEN IN THE  
 COLUMNS OF MATRIX  $V$ . THE EIGENVECTORS OF THE ORIGINAL MATRIX ARE  
 OBTAINED BY MULTIPLYING (OR POSSIBLE INTERCHANGING) THE ROWS OF THE  
 MATRIX  $V$  WITH THE SCALING FACTORS. AS THE SCALING FACTORS ARE REAL  
 QUANTITIES, THE TRANSFORMATION IS PERFORMED BY CALLING THE  
 PROCEDURE BAKLBR FOR BOTH VR AND VI (DEKKER AND HOFFMANN, 1968).

#### REFERENCES:

DEKKER, T.J. AND W. HOFFMANN (1968),  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2,  
 MATH. CENTRE TRACTS 23, MATHEMATISCH CENTRUM;

OSBORNE, E.E. (1960),  
 ON PRECONDITIONING OF MATRICES,  
 JACH., 7, P. 338-354;

PARLETT, B.N. AND C. REINSCH (1969),  
 BALANCING A MATRIX FOR CALCULATION OF EIGENVALUES AND  
 EIGENVECTORS,  
 NUM. MATH., 13, P. 293-304;

## EXAMPLE OF USE:

BAKLBRCOM IS USED IN THE PROCEDURE EIGCOM (SEE SECTION 3.3.2.2.2.). AS A FORMAL TEST OF THE PROCEDURE EQILBRCOM, THE FOLLOWING MATRIX WAS USED:

```

  1      0  1024*I
  0      1      0
I/1024  0      2

```

```

"BEGIN" "INTEGER" I,J;
"REAL" "ARRAY" A1,A2[1:3,1:3],EM[0:7],D,INT[1:3];
"PROCEDURE" INIMAT(LR,UR,LC,UC,A,X);"CODE" 31011;
"PROCEDURE" EQILBRCOM(A1,A2,N,EM,D,INT);"CODE" 34361;
EM[0]:=5"-14;EM[6]:=10;
INIMAT(1,3,1,3,A1,0);INIMAT(1,3,1,3,A2,0);
A1[1,1]:=A1[2,2]:=1;A1[3,3]:=2;
A2[1,3]:=2**10;A2[3,1]:=2**(-10);
EQILBRCOM(A1,A2,3,EM,D,INT);
OUTPUT(61,"("("EQUILIBRATED MATRIX:"),"/")");
OUTPUT(61,"("3(D2B),/,2(D2B),("I"),/,D2B,("I"),2BD/"",
      A1[1,1],A1[1,2],A1[1,3],A1[2,1],A1[2,2],A1[3,1],A1[3,3]);
OUTPUT(61,"(/,("EM[7]:"),5BD/"",EM[7]);
OUTPUT(61,"("D[1:3]:"),3(3ZD2B),/"",D[1],D[2],D[3]);
OUTPUT(61,"("INT[1:3]:"),BD,3B,2BD,4BD)",
      INT[1],INT[2],INT[3])
"END"

```

```

OUTPUT:
EQUILIBRATED MATRIX:
  1  0  0
  0  1  I
  0  I  2

```

```

EM[7]:      4
D[1:3]:    1  1024  1
INT[1:3]:  2      0  0

```

## SOURCE TEXT(S) :

```

"CODE" 34361;
"PROCEDURE" EQILBRCOM(A1, A2, N, EM, D, INT); "VALUE" N;
"INTEGER" N; "ARRAY" A1, A2, EM, D; "INTEGER" "ARRAY" INT;
"BEGIN" "INTEGER" I, P, Q, J, T, COUNT, EXPONENT, NI, IM, I1;
  "REAL" C, R, EPS;
  "PROCEDURE" ICHCOL(L,U,I,J,A);"CODE" 34031;
  "PROCEDURE" ICHROW(L,U,I,J,A);"CODE" 34032;
  "REAL" "PROCEDURE" TAMMAT(L,U,I,J,A,B);"CODE" 34014;
  "REAL" "PROCEDURE" MATTAM(L,U,I,J,A,B);"CODE" 34015;

```

"COMMENT"

```

"PROCEDURE" MOVE(K); "VALUE" K; "INTEGER" K;
"BEGIN" "REAL" DI;
  NI:= Q - P; T:= T + 1; "IF" K # I "THEN"
  "BEGIN" ICHCOL(1, N, K, I, A1); ICHROW(1, N, K, I, A1);
    ICHCOL(1, N, K, I, A2); ICHROW(1, N, K, I, A2);
    DI:= D[I]; D[I]:= D[K]; D[K]:= DI
  "END"
"END" MOVE;
EPS:= EM[0] ** 4; T:= P:= 1; Q:= NI:= I:= N;
COUNT:= EM[6];
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" D[J]:= 1; INT[J]:= 0 "END";
"FOR" I:= "IF" I < Q "THEN" I + 1 "ELSE" P "WHILE" COUNT > 0
"AND" NI > 0 "DO"
"BEGIN" COUNT:= COUNT + 1; IM:= I - 1; I1:= I + 1;
  C:= TAMMAT(P, IM, I, I, A1, A1) + TAMMAT(I1, Q, I,
  I, A1, A1) + TAMMAT(P, IM, I, I, A2, A2) +
  TAMMAT(I1, Q, I, I, A2, A2);
  R:= MATTAM(P, IM, I, I, A1, A1) + MATTAM(I1, Q, I,
  I, A1, A1) + MATTAM(P, IM, I, I, A2, A2) +
  MATTAM(I1, Q, I, I, A2, A2); "IF" C / EPS <= R "THEN"
  "BEGIN" INT[T]:= I; MOVE(P); P:= P + 1 "END"
  "ELSE" "IF" R / EPS <= C "THEN"
  "BEGIN" INT[T]:= I; MOVE(Q); Q:= Q - 1 "END"
  "ELSE"
  "BEGIN" EXPONENT:= LN(R / C) * 0.36067;
    "IF" ABS(EXPONENT) > 1 "THEN"
    "BEGIN" NI:= Q - P; C:= 2 ** EXPONENT;
      D[I]:= D[I] * C;
      "FOR" J:= 1 "STEP" 1 "UNTIL" IM, I1 "STEP" 1
      "UNTIL" N "DO"
      "BEGIN" A1[J, I]:= A1[J, I] * C;
        A1[I, J]:= A1[I, J] / C;
        A2[J, I]:= A2[J, I] * C;
        A2[I, J]:= A2[I, J] / C
      "END"
    "END"
  "ELSE" NI:= NI - 1
"END"
"END";
EM[7]:= EM[6] + COUNT
"END" EQUILBRCOM;
"EOP"

```

```

"CODE" 34362;
"PROCEDURE" BAKLBRCOM(N, N1, N2, D, INT, VR, VI);
"VALUE" N, N1, N2; "INTEGER" N, N1, N2; "ARRAY" D, VR, VI;
"INTEGER" "ARRAY" INT;
"BEGIN"
  "PROCEDURE" BAKLBR(N, N1, N2, D, INT, VEC); "CODE" 34174;
  BAKLBR(N, N1, N2, D, INT, VR);
  BAKLBR(N, N1, N2, D, INT, VI)
"END" BAKLBRCOM;
"EOP"

```



SECTION:3.2.1.2.1.1

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BRIEF DESCRIPTION:

THIS SECTION CONTAINS FIVE PROCEDURES.

A) TFMSYMTRI2 AND TFMSYMTRI1 TRANSFORM A REAL SYMMETRIC MATRIX INTO A SIMILAR TRIDIAGONAL ONE BY MEANS OF HOUSEHOLDER'S TRANSFORMATION,

B) BAKSYMTRI2 AND BAKSYMTRI1 PERFORM THE CORRESPONDING BACK TRANSFORMATION AND FINALLY,

C) TFMPREVEC (WHICH IS TO BE USED IN COMBINATION WITH TFMSYMTRI2) CALCULATES THE TRANSFORMING MATRIX.

TFMSYMTRI2 AND BAKSYMTRI2 USE THE UPPER TRIANGLE OF A TWO-DIMENSIONAL ARRAY FOR THE UPPER TRIANGLE OF THE GIVEN SYMMETRIC MATRIX (TFMSYMTRI2) OR FOR THE DATA FOR HOUSEHOLDER'S BACK TRANSFORMATION (BAKSYMTRI2). THE OTHER ELEMENTS ARE NEITHER USED NOR CHANGED.

TFMSYMTRI1 AND BAKSYMTRI1 USE "ARRAY" FOR THE GIVEN SYMMETRIC MATRIX (TFMSYMTRI1) OR FOR THE DATA FOR HOUSEHOLDER'S TRANSFORMATION (BAKSYMTRI1).

KEYWORDS:

HOUSEHOLDER'S TRANSFORMATION,  
TRIANGULARIZATION.

SUBSECTION: TFMSYMTRI2.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" TFMSYMTRI2(A, N, D, B, BB, EM); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, D, B, BB, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE UPPER TRIANGLE OF THE SYMMETRIC MATRIX MUST BE  
 GIVEN IN THE UPPER TRIANGULAR PART OF A (THE  
 ELEMENTS A[I, J], I ≤ J);  
 EXIT: THE DATA FOR HOUSEHOLDER'S BACK TRANSFORMATION IS  
 DELIVERED IN THE UPPER TRIANGULAR PART OF A. THE  
 ELEMENTS A[I, J], I > J ARE NEITHER USED NOR CHANGED;  
 D: <ARRAY IDENTIFIER>;  
 "ARRAY" D[1:N];  
 EXIT: THE MAIN DIAGONAL OF THE SYMMETRIC TRIDIAGONAL  
 MATRIX T (SAY), PRODUCED BY HOUSEHOLDER'S  
 TRANSFORMATION;  
 B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 EXIT: THE CODIAGONAL ELEMENTS OF T ARE DELIVERED IN B[1]  
 THROUGH B[N-1]; B[N] IS SET EQUAL TO ZERO;  
 BB: <ARRAY IDENTIFIER>;  
 "ARRAY" BB[1:N];  
 EXIT: THE SQUARES OF THE CODIAGONAL ELEMENTS OF T ARE  
 DELIVERED IN BB[1] THROUGH BB[N-1]; BB[N] IS SET  
 EQUAL TO ZERO;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:1];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EXIT: EM[1], THE INFINITY NORM OF THE ORIGINAL MATRIX.

PROCEDURES USED:

TAMVEC	=	CP34012,
MATMAT	=	CP34013,
TAMMAT	=	CP34014,
ELMVECCOL	=	CP34021,
ELMCOLVEC	=	CP34022,
ELMCOL	=	CP34023.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

A GIVEN SYMMETRIC MATRIX M IS TRANSFORMED INTO A TRIDIAGONAL ONE BY MEANS OF  $N-1$  ORTHOGONAL SIMILARITY TRANSFORMATIONS; THE  $P$ -TH TRANSFORMATION IS CHOSEN IN SUCH A WAY THAT IN THE  $(N-P+1)$ -TH COLUMN AND ROW OF M THE DESIRED ZEROES ARE INTRODUCED. HOWEVER, IF, IN THIS COLUMN AND ROW, ALL ELEMENTS OUTSIDE THE MAIN DIAGONAL AND THE ADJACENT CODIAGONALS ARE SMALLER IN ABSOLUTE VALUE THAN THE INFINITY NORM OF M TIMES THE MACHINE PRECISION, THEN THE  $P$ -TH TRANSFORMATION IS SKIPPED.

FOR FURTHER DETAILS SEE REF [1] AND REF [2].

## SUBSECTION: BAKSYMTRIZ.

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" BAKSYMTRIZ(A, N, N1, N2, VEC); "VALUE" N, N1, N2;  
 "INTEGER" N, N1, N2; "ARRAY" A, VEC;

## THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A [1:N, 1:N];  
 ENTRY: THE DATA FOR THE BACK TRANSFORMATION, AS PRODUCED  
 BY TFMSYMTRIZ, MUST BE GIVEN IN THE UPPER  
 TRIANGULAR PART OF A;  
 N1, N2: <ARITHMETIC EXPRESSION>;  
 LOWER AND UPPER BOUND, RESPECTIVELY, OF THE COLUMN NUMBERS  
 OF VEC;  
 VEC: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC [1:N, N1:N2];  
 ENTRY: THE VECTORS ON WHICH THE BACK TRANSFORMATION HAS TO  
 BE PERFORMED;  
 EXIT: THE TRANSFORMED VECTORS.

## PROCEDURES USED:

TAMMAT = CP34014,  
 ELMCOL = CP34023,

RUNNING TIME: ROUGHLY PROPORTIONAL TO  $N$  SQUARED TIMES  $(N2-N1+1)$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE REF [1].

SECTION: 3.2.1.2, 1.1

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SUBSECTION: TFMPREVEC.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:

"PROCEDURE" TFMPREVEC(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;

THE ORDER OF THE MATRIX;

A: <ARRAY IDENTIFIER>;

"ARRAY" A[1:N, 1:N];

ENTRY: THE DATA FOR THE BACK TRANSFORMATION, AS PRODUCED BY TFMSYMRI2, MUST BE GIVEN IN THE UPPER TRIANGULAR PART OF A;

EXIT: THE MATRIX WHICH TRANSFORMS THE ORIGINAL MATRIX INTO A SIMILAR TRIDIAGONAL ONE.

PROCEDURES USED:

TAMMAT = CP34014,

ELMCOL = CP34023.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE REF [1].

SUBSECTION: TFMSYMTRI1.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
 "PROCEDURE" TFMSYMTRI1(A, N, D, B, BB, EM); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, D, B, BB, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:(N+1)\*N//2];  
 ENTRY: THE UPPER TRIANGLE OF THE GIVEN MATRIX MUST BE  
 GIVEN IN SUCH A WAY THAT THE (I,J)-TH ELEMENT OF  
 THE MATRIX IS A[(J-1)\*J//2+I],  $1 \leq I \leq J \leq N$ ;  
 EXIT: THE DATA FOR HOUSEHOLDER'S BACK TRANSFORMATION AS  
 USED BY BAKSYMTRI1;  
 D: <ARRAY IDENTIFIER>;  
 "ARRAY" D[1:N];  
 EXIT: THE MAIN DIAGONAL OF THE SYMMETRIC TRIDIAGONAL  
 MATRIX T (SAY), PRODUCED BY HOUSEHOLDER'S  
 TRANSFORMATION;  
 B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N];  
 EXIT: THE CODIAGONAL ELEMENTS OF T ARE DELIVERED IN B[1]  
 THROUGH B[N-1]; B[N] IS SET EQUAL TO ZERO;  
 BB: <ARRAY IDENTIFIER>;  
 "ARRAY" BB[1:N];  
 EXIT: THE SQUARES OF THE CODIAGONAL ELEMENTS OF T ARE  
 DELIVERED IN BB[1] THROUGH BB[N-1]; BB[N] IS SET  
 EQUAL TO ZERO;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:1];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EXIT: EM[1], THE INFINITY NORM OF THE ORIGINAL MATRIX,

PROCEDURES USED:

VECVEC	=	CP34010,
SEQVEC	=	CP34016,
ELMVEC	=	CP34020,

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE TFMSYMTRI2 (THIS SECTION).

SECTION: 3,2,1,2,1.1

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SUBSECTION: BAKSYMTRI1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" BAKSYMTRI1(A, N, N1, N2, VEC); "VALUE" N, N1, N2;  
 "INTEGER" N, N1, N2; "ARRAY" A, VEC;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:(N+1)\*N//2];  
 ENTRY: THE DATA FOR THE BACK TRANSFORMATION, AS PRODUCED  
 BY TFMSYMTRI1;  
 N1, N2: <ARITHMETIC EXPRESSION>;  
 LOWER AND UPPER BOUND, RESPECTIVELY, OF THE COLUMN NUMBERS  
 OF VEC;  
 VEC: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC[1:N, N1:N2];  
 ENTRY: THE VECTORS ON WHICH THE BACK TRANSFORMATION HAS TO  
 BE PERFORMED;  
 EXIT: THE TRANSFORMED VECTORS.

PROCEDURES USED:

VECVEC = CP34010,  
 ELMVEC = CP34020,

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: AN AUXILIARY ONE-DIMENSIONAL REAL ARRAY OF  
 LENGTH N IS USED.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N SQUARED TIMES (N2-N1+1).

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE REF [1].

REFERENCES:

- [1] DEKKER, T.J. AND HOFFMANN, W.  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2,  
 MATHEMATICAL CENTRE TRACTS 23,  
 MATHEMATISCH CENTRUM, AMSTERDAM, 1968;
- [2] WILKINSON, J.H.  
 THE ALGEBRAIC EIGENVALUE PROBLEM,  
 CLARENDON PRESS, OXFORD 1965.

EXAMPLE OF USE:

THE FIVE PROCEDURES OF THIS SECTION ARE USED IN  
 SECTION 3,3,1,1,2;  
 EIGSYM2 USES TFMSYMTRI2 AND BAKSYMTRI2;  
 EIGSYM1 USES TFMSYMTRI1 AND BAKSYMTRI1;  
 QRISYM USES TFMSYMTRI2 AND TFMPREVEC.

SOURCE TEXT(S):

```

"CODE" 34140;
"COMMENT" MCA 2300;
"PROCEDURE" TFMSYMTRI2(A, N, D, B, BB, EM); "VALUE" N; "INTEGER" N;
"ARRAY" A, B, BB, D, EM;
"BEGIN" "INTEGER" I, J, R, R1;
"REAL" W, X, A1, B0, BB0, D0, MACHTOL, NORM;

"REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B); "CODE" 34014;
"REAL" "PROCEDURE" MATMAT(L, U, I, J, A, B); "CODE" 34013;
"PROCEDURE" ELMVECCOL(L, U, I, A, B, X); "CODE" 34021;
"REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;
"PROCEDURE" ELMCOL(L, U, I, J, A, B, X); "CODE" 34023;
"PROCEDURE" ELMCOLVEC(L, U, I, A, B, X); "CODE" 34022;

NORM:= 0;
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" W:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" J "DO" W:= ABS(A[I,J]) + W;
"FOR" I:= J + 1 "STEP" 1 "UNTIL" N "DO" W:= ABS(A[J,I]) +
W; "IF" W > NORM "THEN" NORM:= W
"END";
MACHTOL:= EM[0] * NORM; EM[1]:= NORM; R:= N;
"FOR" R1:= N - 1 "STEP" -1 "UNTIL" 1 "DO"
"BEGIN" D[R]:= A[R,R]; X:= TAMMAT(1, R - 2, R, R, A, A);
A1:= A[R1,R]; "IF" SQRT(X) <= MACHTOL "THEN"
"BEGIN" B0:= B[R1]:= A1; BB[R1]:= B0 * B0; A[R,R]:= 1 "END"
"ELSE"
"BEGIN" BB0:= BB[R1]:= A1 * A1 + X;
B0:= "IF" A1 > 0 "THEN" -SQRT(BB0) "ELSE" SQRT(BB0);
A1:= A[R1,R]:= A1 - B0; W:= A[R,R]:= 1 / (A1 * B0);
"FOR" J:= 1 "STEP" 1 "UNTIL" R1 "DO" B[J]:= (TAMMAT(1,
J, J, R, A, A) + MATMAT(J + 1, R1, J, R, A, A)) * W;
ELMVECCOL(1, R1, R, B, A, TAMVEC(1, R1, R, A, B) *
W * .5); "FOR" J:= 1 "STEP" 1 "UNTIL" R1 "DO"
"BEGIN" ELMCOL(1, J, J, R, A, A, B[J]);
ELMCOLVEC(1, J, J, A, B, A[J,R])
"END"; B[R1]:= B0
"END"; R:= R1
"END";
D[1]:= A[1,1]; A[1,1]:= 1; B[N]:= BB[N]:= 0
"END" TFMSYMTRI2;
"EOF"

```

```

"CODE" 34141;
"COMMENT" MCA 2301;
"PROCEDURE" BAKSYMTRIZ(A, N, N1, N2, VEC); "VALUE" N, N1, N2;
"INTEGER" N, N1, N2; "ARRAY" A, VEC;
"BEGIN" "INTEGER" I, J, K; "REAL" W;

      "REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B); "CODE" 34014;
      "PROCEDURE" ELMCOL(L, U, I, J, A, B, X); "CODE" 34023;

      "FOR" J:= 2 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" W:= A[J,J]; "IF" W < 0 "THEN"
          "FOR" K:= N1 "STEP" 1 "UNTIL" N2 "DO"
              ELMCOL(1, J - 1, K, J, VEC, A,
                  TAMMAT(1, J - 1, J, K, A, VEC) * W)
          "END"
      "END" BAKSYMTRIZ;
"EOP"

```

```

"CODE" 34142;
"COMMENT" MCA 2302;
"PROCEDURE" TFMPREVEC(A, N); "VALUE" N; "INTEGER" N; "ARRAY" A;
"BEGIN" "INTEGER" I, J, J1, K; "REAL" AB;

      "REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B); "CODE" 34014;
      "PROCEDURE" ELMCOL(L, U, I, J, A, B, X); "CODE" 34023;

      J1:= 1;
      "FOR" J:= 2 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" "FOR" I:= 1 "STEP" 1 "UNTIL" J1 - 1 ,
          J "STEP" 1 "UNTIL" N "DO" A[I,J1]:= 0;
          A[J1,J1]:= 1; AB:= A[J,J];
          "IF" AB < 0 "THEN"
              "FOR" K:= 1 "STEP" 1 "UNTIL" J1 "DO"
                  ELMCOL(1, J1, K, J, A, A,
                      TAMMAT(1, J1, J, K, A, A) * AB); J1:= J
          "END";
      "FOR" I:= N - 1 "STEP" -1 "UNTIL" 1 "DO"
          A[I,N]:= 0; A[N,N]:= 1
      "END" TFMPREVEC;
"EOP"

```



```

"CODE" 34143;
"COMMENT" MCA 2305;
"PROCEDURE" TFMSYMTRI1(A, N, D, B, BB, EM); "VALUE" N; "INTEGER" N;
"ARRAY" A, B, BB, D, EM;
"BEGIN" "INTEGER" I, J, R, R1, P, Q, TI, TJ;
"REAL" S, W, X, A1, B0, BB0, D0, NORM, MACHTOL;

"REAL" "PROCEDURE" VECVEC(L, U, SHIFT, A, B); "CODE" 34010;
"REAL" "PROCEDURE" SEQVEC(L, U, IL, SHIFT, A, B); "CODE" 34016;
"PROCEDURE" ELMVEC(L, U, SHIFT, A, B, X); "CODE" 34020;

NORM:= 0; TJ:= 0;
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
NORM:= 0; TJ:= 0;
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" W:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" J "DO" W:= ABS(A[I + TJ]) + W;
TJ:= TJ + J; TI:= TJ + J;
"FOR" I:= J + 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" W:= ABS(A[TI]) + W; TI:= TI + I "END";
"IF" W > NORM "THEN" NORM:= W
"END";
MACHTOL:= EM[0] * NORM; EM[1]:= NORM; Q:= (N + 1) * N // 2;
R:= N; "FOR" R1:= N - 1 "STEP" -1 "UNTIL" 1 "DO"
"BEGIN" P:= Q - R; D[R]:= A[Q];
X:= VECVEC(P + 1, Q - 2, 0, A, A);
A1:= A[Q - 1]; "IF" SQRT(X) <= MACHTOL "THEN"
"BEGIN" B0:= B[R1]:= A1; BB[R1]:= B0 * B0; A[Q]:= 1 "END"
"ELSE"
"BEGIN" BB0:= BB[R1]:= A1 * A1 + X;
B0:= "IF" A1 > 0 "THEN" -SQRT(BB0) "ELSE" SQRT(BB0);
A1:= A[Q - 1]:= A1 - B0; W:= A[Q]:= 1 / (A1 * B0);
TJ:= 0; "FOR" J:= 1 "STEP" 1 "UNTIL" R1 "DO"
"BEGIN" TI:= TJ + J; S:= VECVEC(TJ + 1, TI, P - TJ,
A, A); TJ:= TI + J;
B[J]:= (SEQVEC(J + 1, R1, TJ, P, A, A) + S) * W;
TJ:= TI
"END";
ELMVEC(1, R1, P, B, A, VECVEC(1, R1, P, B, A) * W * 5);
TJ:= 0; "FOR" J:= 1 "STEP" 1 "UNTIL" R1 "DO"
"BEGIN" TI:= TJ + J; ELMVEC(TJ + 1, TI, P - TJ, A, A,
B[J]); ELMVEC(TJ + 1, TI, -TJ, A, B, A[J + P]);
TJ:= TI
"END"; B[R1]:= B0
"END";
Q:= P; R:= R1
"END";
D[1]:= A[1]; A[1]:= 1; B[N]:= BB[N]:= 0
"END" TFMSYMTRI1;
"EQP"
    
```

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"CODE" 34144;
"COMMENT" MCA 2306;
"PROCEDURE" BAKSYMTRI1(A, N, N1, N2, VEC); "VALUE" N, N1, N2;
"INTEGER" N, N1, N2; "ARRAY" A, VEC;
"BEGIN" "INTEGER" J, J1, K, TI, TJ;
        "REAL" W; "ARRAY" AUXVEC[1:N];

        "REAL" "PROCEDURE" VECVEC(L, U, SHIFT, A, B); "CODE" 34010;
        "PROCEDURE" ELMVEC(L, U, SHIFT, A, B, X); "CODE" 34020;

        "FOR" K:= N1 "STEP" 1 "UNTIL" N2 "DO"
        "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
            AUXVEC[J]:= VEC[J,K]; TJ:= J1:= 1;
            "FOR" J:= 2 "STEP" 1 "UNTIL" N "DO"
                "BEGIN" TI:= TJ + J; W:= A[TI];
                    "IF" W < 0 "THEN" ELMVEC(1, J1, TJ, AUXVEC, A, VECVEC(1,
                        J1, TJ, AUXVEC, A) * W); J1:= J; TJ:= TI
                "END";
            "FOR" J:= 1 "STEP" 1 "UNTIL" N "DO" VEC[J,K]:= AUXVEC[J]
        "END"
"END" BAKSYMTRI1;
"EQP"
  
```

1-st REVISION, 1975



SECTION: 3.2.1.2.1.2

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PAGE 1

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RECEIVED: 731112.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS THREE PROCEDURES.

- A) TFMREAHES TRANSFORMS A MATRIX INTO A SIMILAR UPPER-HESSSENBERG MATRIX BY MEANS OF WILKINSON'S TRANSFORMATION,
- B) BAKREAHES1 PERFORMS THE CORRESPONDING BACK TRANSFORMATION ON A VECTOR AND SHOULD BE CALLED AFTER TFMREAHES,
- C) BAKREAHES2 PERFORMS THE CORRESPONDING BACK TRANSFORMATION ON THE COLUMNS OF A MATRIX AND SHOULD BE CALLED AFTER TFMREAHES.

KEYWORDS:

SIMILARITY TRANSFORMATION,  
UPPER-HESSSENBERG MATRIX.

SECTION: 3.2.1.2.1.2

(DECEMBER 1975)

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SUBSECTION: TFMREAHES.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

```

"PROCEDURE" TFMREAHES(A, N, EM, INT); "VALUE" N;
"INTEGER" N; "ARRAY" A, EM; "INTEGER" "ARRAY" INT;

```

THE MEANING OF THE FORMAL PARAMETERS IS:

```

N:      <ARITHMETIC EXPRESSION>;
        THE ORDER OF THE GIVEN MATRIX;
A:      <ARRAY IDENTIFIER>;
        "ARRAY" A[1:N,1:N];
        ENTRY:  THE MATRIX TO BE TRANSFORMED;
        EXIT:   THE UPPER-HESSSENBERG MATRIX IS DELIVERED IN THE
                UPPER TRIANGLE AND THE FIRST SUBDIAGONAL OF A, THE
                (NONTRIVIAL ELEMENTS OF THE) TRANSFORMING MATRIX,
                L, IN THE REMAINING PART OF A, I.E. A[I,J] =
                L[I,J + 1], FOR I = 3,...,N AND J = 1,...,I - 2;
EM:     <ARRAY IDENTIFIER>;
        "ARRAY" EM[0:1];
        ENTRY:  EM[0], THE MACHINE PRECISION;
        EXIT:   EM[1], THE INFINITY NORM OF THE ORIGINAL MATRIX;
INT:    <ARRAY IDENTIFIER>;
        "INTEGER" "ARRAY" INT[1:N];
        EXIT:   THE PIVOTAL INDICES DEFINING THE STABILIZING ROW
                AND COLUMN INTERCHANGES;

```

PROCEDURES USED:

```

MATVEC      =      CP34011,
MATMAT      =      CP34013,
ICHCOL      =      CP34031,
ICHROW      =      CP34032.

```

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:

A ONE-DIMENSIONAL REAL ARRAY OF LENGTH N IS DECLARED.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

WILKINSON'S TRANSFORMATION IS A TRIANGULAR SIMILARITY TRANSFORMATION WITH STABILIZING ROW AND COLUMN INTERCHANGES TRANSFORMING A MATRIX, M, INTO AN UPPER-HESSSENBERG MATRIX, H. THE TRANSFORMING MATRIX IS THE PRODUCT OF A PERMUTATION MATRIX, P, AND A UNIT LOWER-TRIANGULAR MATRIX, L. THE NONDIAGONAL ELEMENTS IN THE FIRST COLUMN OF L ARE 0, AND THE ROW AND COLUMN INTERCHANGES ARE CHOSEN IN SUCH A WAY THAT THE ABSOLUTE VALUE OF EACH ELEMENT OF L IS AT MOST 1. BECAUSE OF THE SPECIAL FORM OF L, THE MATRICES H AND L CAN BE STORED TOGETHER IN THE ARRAY USED FOR THE MATRIX A (SEE CALLING SEQUENCE). FOR FURTHER DETAILS SEE REFERENCE [1] AND [2].

SUBSECTION: BAKREAHES1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" BAKREAHES1(A, N, INT, V); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, V; "INTEGER" "ARRAY" INT;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE LENGTH OF THE VECTOR TO BE TRANSFORMED;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A [1:N, 1:N];  
 ENTRY: THE (NONTRIVIAL ELEMENTS OF THE) TRANSFORMING  
 MATRIX, L, AS PRODUCED BY TFMREAHES MUST BE GIVEN  
 IN THE PART BELOW THE FIRST SUBDIAGONAL OF A,  
 I.E.  $A[I, J] = L[I, J + 1]$ , FOR  $I = 3, \dots, N$  AND  
 $J = 1, \dots, I - 2$ ;  
 INT: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" INT [1:N];  
 ENTRY: PIVOTAL INDICES DEFINING THE STABILIZING ROW AND  
 COLUMN INTERCHANGES AS PRODUCED BY TFMREAHES;  
 V: <ARRAY IDENTIFIER>;  
 "ARRAY" V [1:N];  
 ENTRY: THE VECTOR TO BE TRANSFORMED;  
 EXIT: THE TRANSFORMED VECTOR.

PROCEDURES USED:

MATVEC = CP34011.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N SQUARED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE BACK TRANSFORMATION WHICH CORRESPONDS TO WILKINSON'S  
 TRANSFORMATION AS PERFORMED BY TFMREAHES TRANSFORMS A VECTOR, X,  
 INTO THE VECTOR PLX, WHERE PL IS THE TRANSFORMING MATRIX.

SUBSECTION: BAKREAHES2,

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" BAKREAHES2(A, N, N1, N2, INT, VEC); "VALUE" N, N1, N2;  
 "INTEGER" N, N1, N2; "ARRAY" A, VEC; "INTEGER" "ARRAY" INT;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE LENGTH OF THE VECTORS TO BE TRANSFORMED;  
 N1, N2: <ARITHMETIC EXPRESSION>;  
 THE COLUMN NUMBERS OF THE FIRST AND LAST VECTOR TO BE  
 TRANSFORMED;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 ENTRY: THE (NONTRIVIAL ELEMENTS OF THE) TRANSFORMING  
 MATRIX, L, AS PRODUCED BY TFMREAHES MUST BE GIVEN  
 IN THE PART BELOW THE FIRST SUBDIAGONAL OF A,  
 I.E.  $A[I, J] = L[I, J + 1]$ , FOR  $I = 3, \dots, N$  AND  
 $J = 1, \dots, I - 2$ ;  
 INT: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" INT[1:N];  
 ENTRY: PIVOTAL INDICES DEFINING THE STABILIZING ROW AND  
 COLUMN INTERCHANGES AS PRODUCED BY TFMREAHES;  
 VEC: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC[1:N, N1:N2];  
 ENTRY: THE  $N2 - N1 + 1$  VECTORS OF LENGTH N TO BE  
 TRANSFORMED;  
 EXIT: THE  $N2 - N1 + 1$  VECTORS OF LENGTH N RESULTING FROM  
 THE BACK TRANSFORMATION;

PROCEDURES USED:

TAMVEC = CP34012,  
 ICHROW = CP34032.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:

IONAL REAL ARRAY OF LENGTH N IS DECLARED.

RUNNING TIME: ROUGHLY PROPORTIONAL TO  $(N2 - N1 + 1) * N * N$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SEE SUBSECTION BAKREAHES1.

REFERENCES:

- [1] DEKKER, T. J. AND HOFFMANN, W.,  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2,  
 MATHEMATICAL CENTRE TRACTS 23,  
 MATHEMATISCH CENTRUM, AMSTERDAM, 1968;
- [2] J. H. WILKINSON, THE ALGEBRAIC EIGENVALUE PROBLEM,  
 CLARENDON PRESS, OXFORD, 1965.

## EXAMPLES OF USE:

EXAMPLES OF USE OF TFMREAHES, BAKREAHES1 AND BAKREAHES2 CAN BE FOUND IN THE PROCEDURES FOR CALCULATING EIGENVALUES AND EIGENVECTORS AS DESCRIBED IN SECTION 3.3.1.2.2.

## SOURCE TEXT(S) :

```

"CODE" 34170;
"COMMENT" MCA 2400;
"PROCEDURE" TFMREAHES(A, N, EM, INT); "VALUE" N; "INTEGER" N;
"ARRAY" A, EM; "INTEGER" "ARRAY" INT;
"BEGIN" "INTEGER" I, J, J1, K, L;
"REAL" S, T, MACHTOL, MACHEPS, NORM;
"ARRAY" B(0:N - 1);

"REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
"REAL" "PROCEDURE" MATMAT(L, U, I, J, A, B); "CODE" 34013;
"PROCEDURE" ICHCOL(L, U, I, J, A); "CODE" 34031;
"PROCEDURE" ICHROW(L, U, I, J, A); "CODE" 34032;

MACHEPS:= EM(0); NORM:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" S:= 0;
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO" S:= S + ABS(A[I,J]);
"IF" S > NORM "THEN" NORM:= S
"END";
EM[1]:= NORM; MACHTOL:= NORM * MACHEPS; INT[1]:= 0;
"FOR" J:= 2 "STEP" 1 "UNTIL" N "DO"
"BEGIN" J1:= J - 1; L:= 0; S:= MACHTOL;
"FOR" K:= J + 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" T:= ABS(A[K,J1]); "IF" T > S "THEN"
"BEGIN" L:= K; S:= T "END"
"END";
"IF" L = 0 "THEN"
"BEGIN" "IF" ABS(A[J,J1]) < S "THEN"
"BEGIN" ICHROW(1, N, J, L, A);
ICHCOL(1, N, J, L, A)
"END"
"ELSE" L:= J; T:= A[J,J1];
"FOR" K:= J + 1 "STEP" 1 "UNTIL" N "DO"
A[K,J1]:= A[K,J1] / T
"END"
"ELSE"
"FOR" K:= J + 1 "STEP" 1 "UNTIL" N "DO" A[K,J1]:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
B[I - 1]:= A[I,J1]; A[I,J1]:= A[I,J] +
("IF" L = 0 "THEN" 0 "ELSE" MATMAT(J + 1, N, I, J1, A, A))-
MATVEC(1, "IF" J1 < I - 2 "THEN" J1 "ELSE" I - 2, I, A, B);
INT[J]:= L
"END"
"END" TFMREAHES;
"EOF"

```

```

"CODE" 34171;
"COMMENT" MCA 2401;
"PROCEDURE" BAKREAHES1(A, N, INT, V); "VALUE" N; "INTEGER" N;
"ARRAY" A, V; "INTEGER" "ARRAY" INT;
"BEGIN" "INTEGER" I, L;
"REAL" W; "ARRAY" X[1:N];

"REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;

"FOR" I:= 2 "STEP" 1 "UNTIL" N "DO" X[I - 1]:= V[I];
"FOR" I:= N "STEP" -1 "UNTIL" 2 "DO"
"BEGIN" V[I]:= V[I] + MATVEC(1, I - 2, I, A, X);
L:= INT[I]; "IF" L > I "THEN"
"BEGIN" W:= V[I]; V[I]:= V[L]; V[L]:= W "END"
"END"
"END" BAKREAHES1;
"EOP"

```

```

"CODE" 34172;
"COMMENT" MCA 2402;
"PROCEDURE" BAKREAHES2(A, N, N1, N2, INT, VEC); "VALUE" N, N1, N2;
"INTEGER" N, N1, N2; "ARRAY" A, VEC; "INTEGER" "ARRAY" INT;
"BEGIN" "INTEGER" I, L, K; "ARRAY" U[1:N];

"REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;
"PROCEDURE" ICHROW(L, U, I, J, A); "CODE" 34032;

"FOR" I:= N "STEP" -1 "UNTIL" 2 "DO"
"BEGIN" "FOR" K:= I - 2 "STEP" -1 "UNTIL" 1 "DO"
U[K + 1]:= A[I, K];
"FOR" K:= N1 "STEP" 1 "UNTIL" N2 "DO"
VEC[I, K]:= VEC[I, K] + TAMVEC(2, I - 1, K, VEC, U);
L:= INT[I]; "IF" L > I "THEN" ICHROW(N1, N2, I, L, VEC)
"END"
"END" BAKREAHES2;
"EOP"

```



SECTION: 3.2.1.2.2.1

(JUNE 1974)

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BRIEF DESCRIPTION :

THIS SECTION CONTAINS THREE PROCEDURES;  
 A) HSHHRMTRI TRANSFORMS THE HERMITIAN MATRIX M INTO A SIMILAR  
 REAL SYMMETRIC TRIDIAGONAL MATRIX S;  
 B) BAKHRMTRI PERFORMS A BACK TRANSFORMATION CORRESPONDING TO  
 HSHHRMTRI;  
 C) HSHHRMTRIVAL DELIVERS THE MAIN DIAGONAL ELEMENTS AND THE  
 SQUARES OF THE CODIAGONAL ELEMENTS OF A HERMITIAN TRIDIAGONAL  
 MATRIX WHICH IS UNITARY SIMILAR WITH A GIVEN HERMITIAN MATRIX.

KEYWORDS :

HERMITIAN MATRIX ,  
 TRIDIAGONALIZATION ,  
 COMPLEX HOUSEHOLDER'S TRANSFORMATION .

SUBSECTION : HSHHRMTRI.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE READS :  
 "PROCEDURE" HSHHRMTRI(A, N, D, B, BB, EM, TR, TI); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, D, B, BB, EM, TR, TI;

THE MEANING OF THE FORMAL PARAMETERS IS :

A, TR, TI: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N, 1:N];  
 "ARRAY" TR, TI[1:N-1];  
 ENTRY: THE REAL PART OF THE UPPER TRIANGLE OF THE  
 HERMITIAN MATRIX MUST BE GIVEN IN THE UPPER  
 TRIANGULAR PART OF A (THE ELEMENTS A[I, J], I ≤ J);  
 THE IMAGINARY PART OF THE STRICT LOWER TRIANGLE  
 OF THE HERMITIAN MATRIX MUST BE GIVEN IN THE  
 STRICT LOWER PART OF A (THE ELEMENTS A[I, J], I > J);  
 EXIT: DATA FOR THE BACKTRANSFORMATION;

```

N:      <ARITHMETIC EXPRESSION>;
        THE ORDER OF THE MATRIX;
D:      <ARRAY IDENTIFIER>;
        "ARRAY"D[1:N];
        EXIT : THE MAIN DIAGONAL OF THE RESULTING SYMMETRIC
                TRIDIAGONAL MATRIX;
B:      <ARRAY IDENTIFIER>;
        "ARRAY"B[1:N-1];
        EXIT: THE CODIAGONAL ELEMENTS OF THE RESULTING SYMMETRIC
                TRIDIAGONAL MATRIX;
BB:     <ARRAY IDENTIFIER>;
        "ARRAY"BB[1:N-1];
        EXIT : THE SQUARES OF THE MODULI OF THE CODIAGONAL
                ELEMENTS OF THE RESULTING SYMMETRIC TRIDIAGONAL
                MATRIX;
EM:     <ARRAY IDENTIFIER>;
        "ARRAY"EM[0:1];
        ENTRY: EM[0], THE MACHINE PRECISION;
        EXIT:  EM[1], AN ESTIMATE FOR A NORM OF THE ORIGINAL
                MATRIX.

```

PROCEDURES USED :

```

MATVEC      = CP34011 .
TAMVEC      = CP34012 .
MATMAT      = CP34013 .
TAMMAT      = CP34014 .
MATTAM      = CP34015 .
ELMVECCOL   = CP34021 .
ELMCOLVEC   = CP34022 .
ELMCOL      = CP34023 .
ELMROW      = CP34024 .
ELMVECROW   = CP34026 .
ELMROWVEC   = CP34027 .
ELMROWCOL   = CP34028 .
ELMCOLROW   = CP34029 .
CARPOL      = CP34344 .

```

RUNNING TIME : PROPORTIONAL TO N CUBED .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE HSHHRMTRIVAL (THIS SECTION).

SUBSECTION : BAKHRMTRI.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE READS :  
 "PROCEDURE" BAKHRMTRI(A, N, N1, N2, VECR, VECI, TR, TI);  
 "VALUE" N, N1, N2; "INTEGER" N, N1, N2;

THE MEANING OF THE FORMAL PARAMETERS IS :

A,TR,TI: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 "ARRAY" TR, TI[1:N-1];  
 ENTRY: THE DATA FOR THE BACKTRANSFORMATION AS PRODUCED  
 BY HSHHRMTRI;  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE MATRIX OF WHICH THE EIGENVECTORS ARE  
 CALCULATED;  
 N1,N2: <ARITHMETIC EXPRESSION>;  
 THE EIGENVECTORS CORRESPONDING TO THE EIGENVALUES WITH  
 INDICES N1,...,N2 ARE TO BE TRANSFORMED;  
 VECR,VECI: <ARRAY IDENTIFIER>;  
 "ARRAY" VECR,VECI[1:N,N1:N2];  
 ENTRY:  
 THE BACK TRANSFORMATION IS PERFORMED ON THE REAL  
 EIGENVECTORS GIVEN IN THE COLUMNS OF ARRAY VECR;  
 EXIT:  
 VECR : REAL PART OF THE TRANSFORMED EIGENVECTORS;  
 VECI : IMAGINARY PART OF THE TRANSFORMED EIGENVECTORS.

PROCEDURES USED :

MATMAT = CP34013 ,  
 TAMMAT = CP34014 ,  
 ELMCOL = CP34023 ,  
 ELMCOLROW = CP34029 ,  
 COMMUL = CP34341 ,  
 COMROWCST = CP34353 .

RUNNING TIME: PROPORTIONAL TO  $(N2-N1+1)*N**2$  ,

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE HSHHRMTRIVAL (THIS SECTION).

SUBSECTION : HSHHRMTRIVAL.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE READS :  
 "PROCEDURE" HSHHRMTRIVAL(A, N, D, BB, EM); "VALUE" N; "INTEGER" N;  
 "ARRAY" A, D, BB, EM;

THE MEANING OF THE FORMAL PARAMETERS IS :

A: <ARRAY IDENTIFIER>;  
 "ARRAY"A[1:N,1:N];  
 ENTRY: THE REAL PART OF THE UPPER TRIANGLE OF THE  
 HERMITIAN MATRIX MUST BE GIVEN IN THE UPPER  
 TRIANGULAR PART OF A (THE ELEMENTS A[I,J], I<=J);  
 THE IMAGINARY PART OF THE STRICT LOWER TRIANGLE  
 OF THE HERMITIAN MATRIX MUST BE GIVEN IN THE  
 STRICT LOWER PART OF A (THE ELEMENTS A[I,J], I>J);  
 THE ELEMENTS OF A ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

D: <ARRAY IDENTIFIER>;  
 "ARRAY"D[1:N];  
 EXIT: THE MAIN DIAGONAL OF THE RESULTING HERMITIAN  
 TRIDIAGONAL MATRIX;

BB: <ARRAY IDENTIFIER>;  
 "ARRAY"BB[1:N-1];  
 EXIT: THE SQUARES OF THE MODULI OF THE CODIAGONAL  
 ELEMENTS OF THE RESULTING HERMITIAN TRIDIAGONAL  
 MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY"EM[0:1];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EXIT: EM[1], AN ESTIMATE FOR A NORM OF THE ORIGINAL  
 MATRIX;

PROCEDURES USED :

MATVEC = CP34011 ,  
 TAMVEC = CP34012 ,  
 MATMAT = CP34013 ,  
 TAMMAT = CP34014 ,  
 MATTAM = CP34015 ,  
 ELMVECCOL = CP34021 ,  
 ELMCOLVEC = CP34022 ,  
 ELMCOL = CP34023 ,  
 ELMROW = CP34024 ,  
 ELMVECROW = CP34026 ,  
 ELMROWVEC = CP34027 ,  
 ELMROWCOL = CP34028 ,  
 ELMCOLROW = CP34029 ,

RUNNING TIME : PROPORTIONAL TO N CUBED .

LANGUAGE : ALGOL 60.

THE FOLLOWING HOLDS FOR THE THREE PROCEDURES :

METHOD AND PERFORMANCE :

HSHHRMTRIVAL TRANSFORMS A HERMITIAN MATRIX INTO A SIMILAR HERMITIAN TRIDIAGONAL MATRIX BY MEANS OF HOUSEHOLDER'S TRANSFORMATION.

HSHHRMTRI TRANSFORMS A HERMITIAN MATRIX INTO A SIMILAR REAL TRIDIAGONAL MATRIX BY MEANS OF HOUSEHOLDER'S TRANSFORMATION FOLLOWED BY A COMPLEX DIAGONAL UNITARY SIMILARITY TRANSFORMATION IN ORDER TO MAKE THE RESULTING TRIDIAGONAL MATRIX REAL SYMMETRIC;

HOUSEHOLDER'S TRANSFORMATION FOR COMPLEX HERMITIAN MATRICES IS A UNITARY SIMILARITY TRANSFORMATION, TRANSFORMING A HERMITIAN MATRIX INTO A SIMILAR COMPLEX TRIDIAGONAL ONE (SEE WILKINSON, 1965, P. 342-343). LET  $M$  BE A GIVEN HERMITIAN MATRIX OF ORDER  $N$ , WITH REAL PART  $M_R$  AND IMAGINARY PART  $M_I$ ,  $P$  THE TRANSFORMING MATRIX AND  $T$  THE RESULTING HERMITIAN TRIDIAGONAL MATRIX. SINCE  $P$  IS UNITARY, WE HAVE  $T = P^H M P$ , WHERE  $^H$  STANDS FOR CONJUGATING AND TRANSPOSING. THE MATRIX  $P$  IS THE PRODUCT OF  $N-2$  HOUSEHOLDER MATRICES, THESE BEING UNITARY HERMITIAN MATRICES OF THE FORM  $I = U^H U / T$ , WHERE  $T$  IS A SCALAR ( $>0$ ), AND  $U$  A COMPLEX VECTOR. THE  $K$ -TH HOUSEHOLDER MATRIX,  $K=1, \dots, N-2$ , IS CHOSEN IN SUCH A WAY THAT THE LAST  $K$  ELEMENTS OF  $U$  VANISH, AND THE DESIRED ZEROS ARE INTRODUCED IN THE  $(N-K+1)$ -TH COLUMN AND ROW OF THE MATRIX  $M$ . HOWEVER, IF THE EUCLIDIAN NORM OF THE FIRST  $N-K-1$  ELEMENTS OF COLUMN  $N-K+1$  OF THE MATRIX  $M$  IS SMALLER THAN THE MACHINE PRECISION TIMES THE INFINITY NORM OF THE MATRIX ( $\text{NORM}(M_R) + \text{NORM}(M_I)$ ), THEN THE  $K$ -TH TRANSFORMATION IS SKIPPED (I.E. THE  $K$ -TH HOUSEHOLDER MATRIX IS REPLACED BY  $I$ ).

THE COMPLEX DIAGONAL SIMILARITY TRANSFORMATION D TRANSFORMS THE HERMITIAN TRIDIAGONAL MATRIX T INTO A REAL SYMMETRIC TRIDIAGONAL MATRIX S (MUELLER, 1966). THE DIAGONAL OF D IS CHOSEN IN SUCH A WAY THAT THE CODIAGONAL ELEMENTS OF T ARE TRANSFORMED INTO THEIR ABSOLUTE VALUES. BAKHRMTRI PERFORMS THE BACK TRANSFORMATION TO REPLACE THE EIGENVECTORS OF THE TRIDIAGONAL SYMMETRIC MATRIX S BY THE EIGENVECTORS OF THE ORIGINAL HERMITIAN MATRIX M. IF X IS AN EIGENVECTOR OF S THEN PDX IS THE CORRESPONDING EIGENVECTOR OF M. STARTING FROM THE VECTOR  $V=DX$ , THE VECTOR PDX IS OBTAINED BY SUCCESSIVELY REPLACING V BY THE K-TH HOUSEHOLDER MATRIX TIMES V, FOR  $K=N-2, \dots, 1$ . THE RESULTING VECTOR V THEN EQUALS PDX.

REFERENCES :

MUELLER, D.J. (1966),  
HOUSEHOLDER'S METHOD FOR COMPLEX MATRICES AND EIGENSYSTEMS OF  
HERMITIAN MATRICES,  
NUMER. MATH., 8, P.72-92;

WILKINSON, J.H. (1965),  
THE ALGEBRAIC EIGENVALUE PROBLEM,  
CLARENDON PRESS, OXFORD.

EXAMPLE OF USE :

THE PROCEDURES HSHHRMTRIVAL AND BAKHRMTRI ARE USED IN SECTION 3.3.2.1. :  
EIGVALHRM AND QRIVALHRM USE HSHHRMTRIVAL,  
EIGHRM AND QRHRM USE BAKHRMTRI .  
AS A FORMAL TEST OF THE PROCEDURE HSHHRMTRI, THE FOLLOWING MATRIX WAS USED (SEE GREGORY AND KARNEY, CHAPTER 6, EXAMPLE 6.6) :

$$\begin{matrix} 3 & 1 & 0 & +2I \\ 1 & 3 & -2I & 0 \\ 0 & +2I & 1 & 1 \\ -2I & 0 & 1 & 1 \end{matrix}$$

```

"BEGIN"
"COMMENT" GREGORY AND KARNEY, CHAPTER 6, EXAMPLE 6.6;
"PROCEDURE" HSHHRMTRI(A,N,D,B,BB,EM,TR,TI); "CODE" 34363;
"PROCEDURE" INIMAT(LR,UR,LC,UC,A,X); "CODE" 31011;
"REAL" "ARRAY" A[1:4,1:4],D,B,BB[1:4],TR,TI[1:3],EM[0:1];
"INTEGER" I,J;
"PROCEDURE" OUT(S,A,N);
"VALUE" N;"INTEGER" N;"ARRAY" A;"STRING" S;
"BEGIN" "INTEGER" I,J;
      OUTPUT(61,("10S"),S);
      "FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
      OUTPUT(61,("+D,3DBB"),A[I]);
      OUTPUT(61,("/"))
"END" OUT;

INIMAT(1,4,1,4,A,0);
A[1,1]:=A[2,2]:=3;
A[1,2]:=A[3,3]:=A[3,4]:=A[4,4]:=1;
A[3,2]:=2;A[4,1]:=-2;
EM[0]:="-14;
OUTPUT(61,(" " ("INITIAL MATRIX GIVEN IN ARRAY A[1:4,1:4]:")",/"));
"FOR" I:=1 "STEP" 1 "UNTIL" 4 "DO"
"BEGIN" "FOR" J:=1 "STEP" 1 "UNTIL" 4 "DO"
      OUTPUT(61,("=DBBB"),A[I,J]);
      OUTPUT(61,("/"))
"END";
OUTPUT(61,("/, ("HSHHRMTRI DELIVERS:")",//"));
HSHHRMTRI(A,4,D,B,BB,EM,TR,TI);
OUT(("D[1:4]: "),D,4);
OUT(("B[1:3]: "),B,3);
OUT(("BB[1:3]: "),BB,3);
OUT(("EM[1]: "),EM,1);
"END"

```

```

OUTPUT :
INITIAL MATRIX GIVEN IN ARRAY A[1:4,1:4]:
  3      1      0      0
  0      3      0      0
  0      2      1      1
 -2      0      0      1

```

HSHHRMTRI DELIVERS:

D[1:4]:	+3,000	+1,400	+2,600	+1,000
B[1:3]:	+2,236	+0,800	+2,236	
BB[1:3]:	+5,000	+0,640	+5,000	
EM[1]:	+6,000			

## SOURCE TEXT(S) :

```

"CODE" 34363;
"PROCEDURE" HSHHRMTRI(A, N, D, B, BB, EM, TR, TI); "VALUE" N;
"INTEGER" N; "ARRAY" A, D, B, BB, EM, TR, TI;
"BEGIN" "INTEGER" I, J, J1, JM1, R, RM1;
  "REAL" NRM, W, TOL2, X, AR, AI, MOD, C, S, H, K, T, Q,
  AJR, ARJ, BJ, BBJ;
  "REAL" "PROCEDURE" MATVEC(L,U,I,A,B); "CODE" 34011;
  "REAL" "PROCEDURE" TAMVEC(L,U,I,A,B); "CODE" 34012;
  "REAL" "PROCEDURE" MATMAT(L,U,I,J,A,B); "CODE" 34013;
  "REAL" "PROCEDURE" TAMMAT(L,U,I,J,A,B); "CODE" 34014;
  "REAL" "PROCEDURE" MATTAM(L,U,I,J,A,B); "CODE" 34015;
  "PROCEDURE" ELMVECCOL(L,U,I,A,B,X); "CODE" 34021;
  "PROCEDURE" ELMCOLVEC(L,U,I,A,B,X); "CODE" 34022;
  "PROCEDURE" ELMCOL(L,U,I,J,A,B,X); "CODE" 34023;
  "PROCEDURE" ELMROW(L,U,I,J,A,B,X); "CODE" 34024;
  "PROCEDURE" ELMVECROW(L,U,I,A,B,X); "CODE" 34026;
  "PROCEDURE" ELMROWVEC(L,U,I,A,B,X); "CODE" 34027;
  "PROCEDURE" ELMROWCOL(L,U,I,J,A,B,X); "CODE" 34028;
  "PROCEDURE" ELMCOLROW(L,U,I,J,A,B,X); "CODE" 34029;
  "PROCEDURE" CARPOL(AR,AI,R,C,S); "CODE" 34344;
  NRM:= 0;
  "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" W:= ABS(A[I,I]);
    "FOR" J:= I - 1 "STEP" - 1 "UNTIL" 1, I + 1 "STEP" 1
    "UNTIL" N "DO" W:= W + ABS(A[I,J]) + ABS(A[J,I]);
    "IF" W > NRM "THEN" NRM:= W
  "END" I;
  TOL2:= (EM[0] * NRM) ** 2; EM[1]:= NRM; R:= N;
  "FOR" RM1:= N - 1 "STEP" - 1 "UNTIL" 1 "DO"
  "BEGIN" X:= TAMMAT(1, R - 2, R, R, A, A) + MATTAM(1, R -
  2, R, R, A, A); AR:= A[RM1,R]; AI:= - A[R, RM1];
  D[R]:= A[R,R]; CARPOL(AR, AI, MOD, C, S);
  "IF" X < TOL2 "THEN"
  "BEGIN" A[R,R]:= - 1; B[RM1]:= MOD;
    BH[RM1]:= MOD * MOD
  "END"

```



```

"ELSE"
"BEGIN" H:= MOD * MOD + X; K:= SQRT(H);
      T:= A[R,R]:= H + MOD * K;
      "IF" AR = 0 "AND" AI = 0 "THEN" A[RM1,R]:= K "ELSE"
      "BEGIN" A[RM1,R]:= AR + C * K;
            A[R,RM1]:= - AI - S * K; S:= - S
      "END";
      C:= - C; J:= 1; JM1:= 0;
      "FOR" J1:= 2 "STEP" 1 "UNTIL" R "DO"
      "BEGIN" B[J]:= (TAMMAT(1, J, J, R, A, A) +
            MATMAT(J1, RM1, J, R, A, A) + MATTAM(1,
            JM1, J, R, A, A) - MATMAT(J1, RM1, R, J,
            A, A)) / T;
            BB[J]:= (MATMAT(1, JM1, J, R, A, A) -
            TAMMAT(J1, RM1, J, R, A, A) - MATMAT(1, J,
            R, J, A, A) - MATTAM(J1, RM1, J, R, A, A))
            / T; JM1:= J; J:= J1
      "END" J1;
      Q:= (TAMVEC(1, RM1, R, A, B) - MATVEC(1, RM1,
      R, A, BB)) / T / 2;
      ELMVECCOL(1, RM1, R, B, A, - Q);
      ELMVECROW(1, RM1, R, BB, A, Q); J:= 1;
      "FOR" J1:= 2 "STEP" 1 "UNTIL" R "DO"
      "BEGIN" AJR:= A[J,R]; ARJ:= A[R,J]; BJ:= B[J];
            BBJ:= BB[J];
            ELMROWVEC(J, RM1, J, A, B, - AJR);
            ELMROWVEC(J, RM1, J, A, BB, ARJ);
            ELMROWCOL(J, RM1, J, R, A, A, - BJ);
            ELMROW(J, RM1, J, R, A, A, BBJ);
            ELMCOLVEC(J1, RM1, J, A, B, - ARJ);
            ELMCOLVEC(J1, RM1, J, A, BB, - AJR);
            ELMCOL(J1, RM1, J, R, A, A, BBJ);
            ELMCOLROW(J1, RM1, J, R, A, A, BJ); J:= J1;
      "END" J1;
      BB[RM1]:= H; B[RM1]:= K;
      "END";
      TR[RM1]:= C; TI[RM1]:= S; R:= RM1;
      "END" RM1;
      D[1]:= A[1,1];
      "END" HSHHRMTRI;
      "EOP"
    
```

```

"CODE" 34365;
"PROCEDURE" BAKHRMTRI(A, N, N1, N2, VECR, VECI, TR, TI);
"VALUE" N, N1, N2; "INTEGER" N, N1, N2;
"ARRAY" A, VECR, VECI, TR, TI;
"BEGIN" "INTEGER" I, J, R, RM1;
  "REAL" C, S, T, QR, QI;
  "REAL" "PROCEDURE" MATMAT(L,U,I,J,A,B);"CODE" 34013;
  "REAL" "PROCEDURE" TAMMAT(L,U,I,J,A,B);"CODE" 34014;
  "PROCEDURE" ELMCOL(L,U,I,J,A,B,X);"CODE" 34023;
  "PROCEDURE" ELMCOLROW(L,U,I,J,A,B,X);"CODE" 34029;
  "PROCEDURE" COMMUL(AR,AI,BR,BI,RR,RI);"CODE" 34341;
  "PROCEDURE" COMROWCST(L,U,I,AR,AI,XR,XI);"CODE" 34353;
  "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
  "FOR" J:= N1 "STEP" 1 "UNTIL" N2 "DO" VECI[I,J]:= 0; C:= 1;
  S:= 0;
  "FOR" J:= N - 1 "STEP" - 1 "UNTIL" 1 "DO"
  "BEGIN" COMMUL(C, S, TR[J], TI[J], C, S);
    COMROWCST(N1, N2, J, VECR, VECI, C, S)
  "END" J;
  RM1:= 2;
  "FOR" R:= 3 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" T:= A[R,R]; "IF" T > 0 "THEN"
    "FOR" J:= N1 "STEP" 1 "UNTIL" N2 "DO"
    "BEGIN" QR:= (TAMMAT(1, RM1, R, J, A, VECR) -
      MATMAT(1, RM1, R, J, A, VECI)) / T;
      QI:= (TAMMAT(1, RM1, R, J, A, VECI) +
      MATMAT(1, RM1, R, J, A, VECR)) / T;
      ELMCOL(1, RM1, J, R, VECR, A, - QR);
      ELMCOLROW(1, RM1, J, R, VECR, A, - QI);
      ELMCOLROW(1, RM1, J, R, VECI, A, QR);
      ELMCOL(1, RM1, J, R, VECI, A, - QI)
    "END";
    RM1:= R;
  "END" R
"END" BAKHRMTRI;
"EOF"

```

```

"CODE" 34364;
"PROCEDURE" HSHHRMTRIVAL(A, N, D, BB, EM); "VALUE" N; "INTEGER" N;
"ARRAY" A, D, BB, EM;
"BEGIN" "INTEGER" I, J, J1, JM1, R, RM1;
"REAL" NRM, W, TOL2, X, AR, AI, H, T, G, AJR, ARJ, DJ,
BBJ, MOD2;
"REAL" "PROCEDURE" MATVEC(L,U,I,A,B); "CODE" 34011;
"REAL" "PROCEDURE" TAMVEC(L,U,I,A,B); "CODE" 34012;
"REAL" "PROCEDURE" MATMAT(L,U,I,J,A,B); "CODE" 34013;
"REAL" "PROCEDURE" TAMMAT(L,U,I,J,A,B); "CODE" 34014;
"REAL" "PROCEDURE" MATTAM(L,U,I,J,A,B); "CODE" 34015;
"PROCEDURE" ELMVECCOL(L,U,I,A,B,X); "CODE" 34021;
"PROCEDURE" ELMCOLVEC(L,U,I,A,B,X); "CODE" 34022;
"PROCEDURE" ELMCOL(L,U,I,J,A,B,X); "CODE" 34023;
"PROCEDURE" ELMROW(L,U,I,J,A,B,X); "CODE" 34024;
"PROCEDURE" ELMVECROW(L,U,I,A,B,X); "CODE" 34026;
"PROCEDURE" ELMROWVEC(L,U,I,A,B,X); "CODE" 34027;
"PROCEDURE" ELMROWCOL(L,U,I,J,A,B,X); "CODE" 34028;
"PROCEDURE" ELMCOLROW(L,U,I,J,A,B,X); "CODE" 34029;
NRM:= 0;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" W:= ABS(A[I,I]);
"FOR" J:= I + 1 "STEP" 1 "UNTIL" 1, I + 1 "STEP" 1
"UNTIL" N "DO" W:= W + ABS(A[I,J]) + ABS(A[J,I]);
"IF" W > NRM "THEN" NRM:= W
"END" I;
TOL2:= (EM[0] * NRM) ** 2; EM[1]:= NRM; R:= N;
"FOR" RM1:= N - 1 "STEP" 1 "UNTIL" 1 "DO"
"BEGIN" X:= TAMMAT(1, R - 2, R, R, A, A) + MATTAM(1, R -
2, R, R, A, A); AR:= A[RM1,R]; AI:= - A[R, RM1];
DIR:= A[R,R];
"IF" X < TOL2 "THEN" BB[RM1]:= AR * AR + AI * AI "ELSE"
"BEGIN" MOD2:= AR * AR + AI * AI; "IF" MOD2 = 0 "THEN"
"BEGIN" A[RM1,R]:= SQRT(X); T:= X "END"
"ELSE"
"BEGIN" X:= X + MOD2; H:= SQRT(MOD2 * X);
T:= X + H; H:= 1 + X / H;
A[R, RM1]:= - AI * H; A[RM1, R]:= AR * H;
"END";
"COMMENT"

```

```

J:= 1; JM1:= 0;
"FOR" J1:= 2 "STEP" 1 "UNTIL" R "DO"
"BEGIN" D[J]:= (TAMMAT(1, J, J, R, A, A) +
MATMAT(J1, RM1, J, R, A, A) + MATTAM(1,
JM1, J, R, A, A) - MATMAT(J1, RM1, R, J,
A, A)) / T;
BB[J]:= (MATMAT(1, JM1, J, R, A, A) -
TAMMAT(J1, RM1, J, R, A, A) - MATMAT(1, J,
R, J, A, A) - MATTAM(J1, RM1, J, R, A, A))
/ T; JM1:= J; J:= J1
"END" J1;
Q:= (TAMVEC(1, RM1, R, A, D) - MATVEC(1, RM1,
R, A, BB)) / T / 2;
ELMVECCOL(1, RM1, R, D, A, - Q);
ELMVECROW(1, RM1, R, BB, A, Q); J:= 1;
"FOR" J1:= 2 "STEP" 1 "UNTIL" R "DO"
"BEGIN" AJR:= A[J,R]; ARJ:= A[R,J]; DJ:= D[J];
BBJ:= BB[J];
ELMROWVEC(J, RM1, J, A, D, - AJR);
ELMROWVEC(J, RM1, J, A, BB, ARJ);
ELMROWCOL(J, RM1, J, R, A, A, - DJ);
ELMROW(J, RM1, J, R, A, A, BBJ);
ELMCOLVEC(J1, RM1, J, A, D, - ARJ);
ELMCOLVEC(J1, RM1, J, A, BB, - AJR);
ELMCOL(J1, RM1, J, R, A, A, BBJ);
ELMCOLROW(J1, RM1, J, R, A, A, DJ); J:= J1;
"END" J1;
BB[RM1]:= X;
"END";
R:= RM1;
"END" RM1;
D[1]:= A[1,1];
"END" HSHHRMTRIVAL;
"EOP"

```

SECTION:3.2.1.2.2.2

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PAGE 1

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RECEIVED: 731016.

BRIEF DESCRIPTION :

THIS SECTION CONTAINS THE PROCEDURES HSHCOMHES AND BAKCOMHES.  
 HSHCOMHES TRANSFORMS A COMPLEX MATRIX BY MEANS OF HOUSEHOLDER'S  
 TRANSFORMATION FOLLOWED BY A COMPLEX DIAGONAL TRANSFORMATION INTO  
 A SIMILAR UNITARY UPPER-HESSSENBERG MATRIX WITH A REAL NONNEGATIVE  
 SUBDIAGONAL.  
 BAKCOMHES PERFORMS THE CORRESPONDING BACK TRANSFORMATION.

KEYWORDS:

COMPLEX EIGENPROBLEM,  
 REDUCTION HESSENBERG FORM,  
 HOUSEHOLDER'S TRANSFORMATION.

SUBSECTION: HSHCOMHES.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "PROCEDURE" HSHCOMHES(AR, AI, N, EM, B, TR, TI, DEL); "VALUE" N;  
 "INTEGER" N; "ARRAY" AR, AI, EM, B, TR, TI, DEL;

THE MEANING OF THE FORMAL PARAMETERS IS:

AR, AI: <ARRAY IDENTIFIER>;  
 "ARRAY" AR, AI[1:N, 1:N];  
 ENTRY:  
 THE REAL PART AND THE IMAGINARY PART OF THE MATRIX TO BE  
 TRANSFORMED MUST BE GIVEN IN THE ARRAYS AR AND AI,  
 RESPECTIVELY;  
 EXIT:  
 THE REAL PART AND THE IMAGINARY PART OF THE UPPER  
 TRIANGLE OF THE RESULTING UPPER-HESSSENBERG MATRIX ARE  
 DELIVERED IN THE CORRESPONDING PARTS OF THE ARRAYS AR  
 AND AI, RESPECTIVELY; DATA FOR THE HOUSEHOLDER BACK-  
 TRANSFORMATION ARE DELIVERED IN THE STRICT LOWER  
 TRIANGLES OF THE ARRAYS AR AND AI;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY"EM[0:1];  
 ENTRY:  
 EM[0]: THE MACHINE PRECISION;  
 EM[1]: AN ESTIMATE OF THE NORM OF THE COMPLEX MATRIX;  
 (OR, E.G. THE SUM OF THE INFINITY NORMS OF THE REAL  
 (PART AND IMAGINARY PART OF THE MATRIX));

B: <ARRAY IDENTIFIER>;  
 "ARRAY"B[1:N-1];  
 EXIT:  
 THE REAL NONNEGATIVE SUBDIAGONAL OF THE RESULTING  
 UPPER-HESSSENBERG MATRIX;

TR, TI: <ARRAY IDENTIFIER>;  
 "ARRAY" TR, TI[1:N];  
 EXIT:  
 THE REAL PART AND THE IMAGINARY PART OF THE DIAGONAL  
 ELEMENTS OF A DIAGONAL SIMILARITY TRANSFORMATION ARE  
 DELIVERED IN THE ARRAYS TR AND TI, RESPECTIVELY; BY THIS  
 INFORMATION THE COMPLEX UPPER-HESSSENBERG MATRIX IS  
 TRANSFORMED INTO A UPPER-HESSSENBERG MATRIX WITH A REAL  
 SUBDIAGONAL;

DEL: <ARRAY IDENTIFIER>;  
 "ARRAY"DEL[1:N-2];  
 EXIT:  
 INFORMATION CONCERNING THE SEQUENCE OF HOUSEHOLDER  
 MATRICES.

PROCEDURES USED:

HSHCOMCOL = CP34355,  
 MATMAT = CP34013,  
 ELMROWCOL = CP34028,  
 HSHCOMPRD = CP34356,  
 CARPOL = CP34344,  
 COMMUL = CP34341,  
 COMCOLCST = CP34352,  
 COMROWCST = CP34353.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE BAKCOMHES (THIS SECTION).

SUBSECTION: BAKCOMHES,

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "PROCEDURE" BAKCOMHES(AR, AI, TR, TI, DEL, VR, VI, N, N1, N2);  
 "VALUE" N, N1, N2; "INTEGER" N, N1, N2;  
 "ARRAY" AR, AI, TR, TI, DEL, VR, VI;

THE MEANING OF THE FORMAL PARAMETERS IS:

AR, AI, TR, TI, DEL:

<ARRAY IDENTIFIER>;  
 "ARRAY" AR, AI[1:N, 1:N];  
 "ARRAY" TR, TI[1:N];  
 "ARRAY" DEL[1:N-2];

ENTRY: THE DATA FOR THE BACKTRANSFORMATION AS PRODUCED  
 BY HSHCOMHES;

VR, VI:

<ARRAY IDENTIFIER>;  
 "ARRAY" VR, VI[1:N, N1:N2];

ENTRY:

THE BACK TRANSFORMATION IS PERFORMED ON THE EIGENVECTORS  
 WITH THE REAL PARTS GIVEN IN ARRAY VR AND THE IMAGINARY  
 PARTS GIVEN IN ARRAY VI;

EXIT:

THE REAL PARTS AND IMAGINARY PARTS OF THE RESULTING  
 EIGENVECTORS ARE DELIVERED IN THE COLUMNS OF THE ARRAYS  
 VR AND VI, RESPECTIVELY;

N:

<ARITHMETIC EXPRESSION>;

THE ORDER OF THE MATRIX OF WHICH THE EIGENVECTORS ARE  
 CALCULATED;

N1, N2:

<ARITHMETIC EXPRESSION>;

THE EIGENVECTORS CORRESPONDING TO THE EIGENVALUES WITH  
 INDICES N1, ..., N2 ARE TO BE TRANSFORMED;

PROCEDURES USED:

COMROWCST = CP34353,  
 HSHCOMPRD = CP34356.

RUNNING TIME: PROPORTIONAL TO  $(N2-N1) * N^{**2}$ .

LANGUAGE : ALGOL 60.

THE FOLLOWING HOLDS FOR BOTH PROCEDURES:

METHOD AND PERFORMANCE:

HSHCOMHES:

HOUSEHOLDER'S TRANSFORMATION (FOR COMPLEX MATRICES) IS A UNITARY SIMILARITY TRANSFORMATION, WHICH TRANSFORMS A COMPLEX MATRIX INTO A SIMILAR UPPER-HESSSENBERG MATRIX (SEE WILKINSON, 1965, P. 347-349). LET  $M$  BE A GIVEN COMPLEX MATRIX OF ORDER  $N$ ,  $P$  THE TRANSFORMING MATRIX AND  $H$  THE RESULTING UPPER-HESSSENBERG MATRIX, SINCE  $P$  IS UNITARY, WE THEN HAVE  $H = P' M P$ , WHERE  $'$  STANDS FOR CONJUGATING AND TRANSPOSING. THE MATRIX  $P$  IS THE PRODUCT OF  $N-2$  HOUSEHOLDER MATRICES, THESE BEING UNITARY HERMITEAN MATRICES OF THE FORM  $I - U U' / T$ , WHERE  $T$  IS A SCALAR ( $>0$ ), AND  $U$  A COMPLEX VECTOR. THE  $R$ -TH HOUSEHOLDER MATRIX,  $R=1, \dots, N-2$ , IS CHOSEN IN SUCH A WAY THAT THE FIRST  $R$  ELEMENTS OF  $U$  VANISH, AND THE DESIRED ZEROS ARE INTRODUCED IN THE LAST  $N-R-1$  ELEMENTS OF THE  $R$ -TH COLUMN OF THE MATRIX  $M$ . HOWEVER, IF THE EUCLIDEAN NORM OF THE LAST  $N-R-1$  ELEMENTS OF COLUMN  $R$  OF THE MATRIX  $M$  IS SMALLER THAN THE MACHINE PRECISION TIMES A NORM OF THE MATRIX THEN THE  $R$ -TH TRANSFORMATION IS SKIPPED (I.E. THE  $R$ -TH HOUSEHOLDER MATRIX IS REPLACED BY  $I$ ). THE COMPLEX DIAGONAL SIMILARITY TRANSFORMATION  $D$  TRANSFORMS THE UPPER-HESSSENBERG MATRIX  $H$  INTO AN UPPER-HESSSENBERG MATRIX  $H_R$ , WITH REAL NONNEGATIVE ELEMENTS. THE DIAGONAL OF  $D$  IS CHOSEN IN SUCH A WAY THAT SUBDIAGONAL ELEMENTS OF  $H$  ARE TRANSFORMED INTO THEIR ABSOLUTE VALUES (SEE MUELLER, 1966).

BAKCOMHES:

THE BACK TRANSFORMATION TRANSFORMS A COMPLEX VECTOR  $X$  INTO THE COMPLEX VECTOR  $PDX$ . IF  $X$  IS AN EIGENVECTOR OF  $H$  THEN  $PDX$  IS THE CORRESPONDING EIGENVECTOR OF  $M$ . STARTING FROM THE VECTOR  $V=DX$ , THE VECTOR  $PDX$  IS OBTAINED BY SUCCESSIVELY REPLACING  $V$  BY THE  $R$ -TH HOUSEHOLDER MATRIX TIMES  $V$ , FOR  $R=N-2, \dots, 1$ . THE RESULTING VECTOR THEN EQUALS  $PDX$ .

REFERENCES:

- MUELLER, D.J. (1966),  
HOUSEHOLDER'S METHOD FOR COMPLEX MATRICES AND EIGENSYSTEMS OF  
HERMITIAN MATRICES,  
NUMER.MATH., 8, P.72-92;
- WILKINSON, J.H. (1965),  
THE ALGEBRAIC EIGENVALUE PROBLEM,  
CLARENDON PRESS, OXFORD;

EXAMPLE OF USE:

HSHCOMHES IS USED IN THE PROCEDURES EIGVALCOM AND EIGCOM,  
BAKCOMHES IS USED IN THE PROCEDURE EIGCOM,  
(SEE SECTION 3.3.2.2.2.).



## SOURCE TEXT(S) :

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"CODE" 34366;
"PROCEDURE" HSHCOMHES(AR, AI, N, EM, B, TR, TI, DEL); "VALUE" N;
"INTEGER" N; "ARRAY" AR, AI, EM, B, TR, TI, DEL;
"BEGIN" "INTEGER" R, RM1, I, J, NM1;
"REAL" TOL, T, XR, XI;
"REAL" "PROCEDURE" MATMAT(L,U,I,J,A,B); "CODE" 34013;
"PROCEDURE" ELMROWCOL(L,U,I,J,A,B,X); "CODE" 34028;
"PROCEDURE" HSHCOMPRD(I,II,L,U,J,AR,AI,BR,BI,T); "CODE" 34356;
"PROCEDURE" COMCOLCST(L,U,J,AR,AI,XR,XI); "CODE" 34352;
"PROCEDURE" COMROWCST(L,U,I,AR,AI,XR,XI); "CODE" 34353;
"PROCEDURE" CARPOL(AR,AI,R,C,S); "CODE" 34344;
"PROCEDURE" COMMUL(AR,AI,BR,BI,RR,RI); "CODE" 34341;
"BOOLEAN" "PROCEDURE" HSHCOMCOL(L,U,J,AR,AI,TOL,K,C,S,T);
"CODE" 34355;
NM1:= N - 1; TOL:= (EM[0] * EM[1]) ** 2; RM1:= 1;
"FOR" R:= 2 "STEP" 1 "UNTIL" NM1 "DO"
"BEGIN" "IF" HSHCOMCOL(R, N, RM1, AR, AI, TOL, B[RM1],
TR[R], TI[R], T) "THEN"
"BEGIN" "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" XR:= (MATMAT(R, N, I, RM1, AI, AI) -
MATMAT(R, N, I, RM1, AR, AR)) / T;
XI:= (MATMAT(R, N, I, RM1, AR, AI) -
MATMAT(R, N, I, RM1, AI, AR)) / T;
ELMROWCOL(R, N, I, RM1, AR, AR, XR);
ELMROWCOL(R, N, I, RM1, AR, AI, XI);
ELMROWCOL(R, N, I, RM1, AI, AR, XI);
ELMROWCOL(R, N, I, RM1, AI, AI, - XR)
"END";
HSHCOMPRD(R, N, R, N, RM1, AR, AI, AR, AI, T);
"END";
DEL[RM1]:= T; RM1:= R
"END" FORR;
"IF" N > 1 "THEN" CARPOL(AR[N,NM1], AI[N,NM1], B[NM1],
TR[N], TI[N]); RM1:= 1; TR[1]:= 1; TI[1]:= 0;
"FOR" R:= 2 "STEP" 1 "UNTIL" N "DO"
"BEGIN" COMMUL(TR[RM1], TI[RM1], TR[R], TI[R], TR[R],
TI[R]); COMCOLCST(1, RM1, R, AR, AI, TR[R], TI[R]);
COMROWCST(R + 1, N, R, AR, AI, TR[R], - TI[R]);
RM1:= R
"END";
"END" HSHCOMHES;
"EOP"
    
```

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"CODE" 34367;
"PROCEDURE" BAKCOMHES(AR, AI, TR, TI, DEL, VR, VI, N, N1, N2);
"VALUE" N, N1, N2; "INTEGER" N, N1, N2;
"ARRAY" AR, AI, TR, TI, DEL, VR, VI;
"BEGIN" "INTEGER" I, R, RM1;
  "REAL" H;
  "PROCEDURE" HSHCOMPRD(I, II, L, U, J, AR, AI, BR, BI, T); "CODE" 34356;
  "PROCEDURE" COMROWCST(L, U, I, AR, AI, XR, XI); "CODE" 34353;
  "FOR" I:= 2 "STEP" 1 "UNTIL" N "DO" COMROWCST(N1, N2, I, VR,
VI, TR[I], TI[I]); R:= N - 1;
  "FOR" RM1:= N - 2 "STEP" - 1 "UNTIL" 1 "DO"
  "BEGIN" H:= DEL[RM1];
    "IF" H > 0 "THEN" HSHCOMPRD(R, N, N1, N2, RM1, VR, VI,
    AR, AI, H); R:= RM1
  "END"
"END" BAKCOMHES;
"EOP"

```

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BRIEF DESCRIPTION :

THIS SECTION CONTAINS THREE PROCEDURES :

1. HSHREABID.  
THIS PROCEDURE TRANSFORMS A GIVEN MATRIX TO BIDIAGONAL FORM, BY PREMULTIPLYING AND POSTMULTIPLYING THE GIVEN MATRIX WITH ORTHOGONAL MATRICES.
2. PSTTFMMAT.  
THIS PROCEDURE CALCULATES THE POSTMULTIPLYING MATRIX FROM THE DATA GENERATED BY HSHREABID.
3. PRETFMMAT.  
THIS PROCEDURE CALCULATES THE PREMULTIPLYING MATRIX FROM THE DATA GENERATED BY HSHREABID.

KEYWORDS :

HOUSEHOLDER'S TRANSFORMATION  
BIDIAGONALISATION

SUBSECTION : HSHREABID

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"PROCEDURE" HSHREABID(A, M, N, D, B, EM);  
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, D, B, EM;

THE MEANING OF THE FORMAL PARAMETERS IS :

A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1:M,1:N];  
ENTRY: THE GIVEN MATRIX;  
EXIT: DATA CONCERNING THE PREMULTIPLYING AND POSTMULTIPLYING MATRICES;

M: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF ROWS OF THE GIVEN MATRIX;

N: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF COLUMNS OF THE GIVEN MATRIX,  
N SHOULD SATISFY  $N \leq M$ ;

D: <ARRAY IDENTIFIER>;  
"ARRAY" D[1:N];  
EXIT: THE DIAGONAL OF THE BIDIAGONAL MATRIX;

B: <ARRAY IDENTIFIER>;  
"ARRAY" B[1:N];  
EXIT: THE SUPERDIAGONAL OF THE BIDIAGONAL MATRIX IS DELIVERED IN B[1:N-1];

EM: <ARRAY IDENTIFIER>;  
"ARRAY" EM[0:1];  
ENTRY: EM[0]: THE MACHINE-PRECISION;  
EXIT: EM[1]: THE INFINITY NORM OF THE GIVEN MATRIX.

PROCEDURES USED :

TAMMAT = CP34014  
MATTAM = CP34015  
ELMCOL = CP34023  
ELMROW = CP34024

RUNNING TIME :

RUNNING TIME IS ROUGHLY PROPORTIONAL TO  $(M + N) * N * N$

METHOD AND PERFORMANCE :

LET US ASSUME A GIVEN MATRIX  $A [ 1:M, 1:N ]$ , WITH  $M \geq N$ .  
FIRSTLY WE PREMULTIPLY A WITH A HOUSEHOLDER MATRIX, CHOSEN IN SUCH  
A WAY THAT THE FIRST COLUMN OF THE RESULTING MATRIX  $A'$  IS ZERO WITH  
THE EXCEPTION OF THE FIRST ELEMENT. SECONDLY WE POSTMULTIPLY  $A'$   
WITH A HOUSEHOLDER MATRIX SO THAT THE FIRST ROW OF THE RESULTING  
MATRIX IS ZERO WITH THE EXCEPTION OF THE FIRST TWO ELEMENTS.  
NOW WE REMOVE THE FIRST ROW AND COLUMN, AND REPEAT THIS PROCESS  
UNTIL THE MATRIX IS TOTALLY TRANSFORMED TO BIDIAGONAL FORM.  
THIS PROCEDURE IS A REWRITING OF A PART OF THE PROCEDURE SVD  
PUBLISHED BY G.H.GOLUB AND C.REINSCH[1]. HOWEVER IN CONTRAST TO  
THEIR PROCEDURE, HERE WE SKIP A TRANSFORMATION IF THE COLUMN OR ROW  
ON WHICH OUR ATTENTION IS FOCUSED IS ALREADY (NEARLY) IN THE  
DESIRED FORM, I.E. IF THE SUM OF THE SQUARES OF THE ELEMENTS THAT  
OUGHT TO BE ZERO IS SMALLER THAN A CERTAIN CONSTANT, IN SVD THE  
TRANSFORMATION IS SKIPPED ONLY IF THE NORM OF THE FULL ROW OR  
COLUMN IS SMALL ENOUGH. OUR WAY SEEMS TO GIVE BETTER RESULTS, AS  
SOME ILL-DEFINED TRANSFORMATIONS ARE SKIPPED. MOREOVER, IF A  
TRANSFORMATION IS SKIPPED, WE DO NOT STORE A ZERO IN THE  
DIAGONAL OR SUPERDIAGONAL, BUT WE STORE THE VALUE THAT WOULD  
HAVE BEEN FOUND IF THE COLUMN OR ROW WAS IN THE DESIRED FORM  
ALREADY.

LANGUAGE : ALGOL-60

SUBSECTION : PSTTFMMAT

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :  
"PROCEDURE" PSTTFMMAT(A, N, V, B);  
"VALUE" N; "INTEGER" N; "ARRAY" A, V, B;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
"ARRAY"A[1:N,1:N];  
THE DATA CONCERNING THE POSTMULTIPLYING MATRIX, AS GENERATED  
BY HSHREABID;  
N: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF COLUMNS AND ROWS OF A;  
V: <ARRAY IDENTIFIER>;  
"ARRAY"V[1:N,1:N];  
EXIT: THE POSTMULTIPLYING MATRIX;  
B: <ARRAY IDENTIFIER>;  
"ARRAY"B[1:N];  
THE SUPERDIAGONAL AS GENERATED BY HSHREABID.

PROCEDURES USED :

MATMAT = CP34013  
ELMCOL = CP34023

RUNNING TIME :

THE RUNNING TIME IS ABOUT PROPORTIONAL TO  $N^{**}3$

LANGUAGE : ALGOL 60

SUBSECTION : PRETFMMAT

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :  
"PROCEDURE" PRETFMMAT(A, M, N, D);  
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, D;

THE MEANING OF THE FORMAL PARAMETERS IS :

A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1:M,1:N];  
ENTRY: THE DATA CONCERNING THE PREMULTIPLYING MATRIX AS  
GENERATED BY HSHREABID  
EXIT : THE PREMULTIPLYING MATRIX.  
M: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF ROWS OF A.  
N: <ARITHMETIC EXPRESSION>;  
THE NUMBER OF COLUMNS OF A, N SHOULD SATISFY  $N \leq M$ .  
D: <ARRAY IDENTIFIER>;  
"ARRAY" D[1:N];  
THE DIAGONAL AS GENERATED BY HSHREABID.

PROCEDURES USED :

TAMMAT = CP34014  
ELMCOL = CP34023

RUNNING TIME :

THE RUNNING TIME IS ABOUT PROPORTIONAL TO  $M * N * N$

LANGUAGE : ALGOL-60

REFERENCES :

[1] WILKINSON, J.H. AND C.REINSCH  
HANDBOOK FOR AUTOMATIC COMPUTATION, VOL. 2  
LINEAR ALGEBRA  
HEIDELBERG (1971)

EXAMPLE OF USE :

FOR AN EXAMPLE OF USE ONE IS REFERRED TO SECTION 3.5.1.2

SOURCE TFX(T(S) :

```

"CODE" 34260;
"PROCEDURE" HSHREABID(A, M, N, D, B, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, D, B, EM;
"BEGIN" "INTEGER" I, J, I1;
  "REAL" NORM, MACHTOL, W, S, F, G, H;

  "REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B);
  "VALUE" L, U, I, J; "INTEGER" L, U, I, J; "ARRAY" A, B;
  "CODE" 34014;
  "REAL" "PROCEDURE" MATTAM(L, U, I, J, A, B);
  "VALUE" L, U, I, J; "ARRAY" A, B;
  "CODE" 34015;

  "PROCEDURE" ELMCOL(L, U, I, J, A, B, X);
  "VALUE" L, U, I, J, X; "INTEGER" L, U, I, J; "REAL" X;
  "ARRAY" A, B;
  "CODE" 34023;
  "PROCEDURE" ELMROW(L, U, I, J, A, B, X);
  "VALUE" L, U, I, J, X; "INTEGER" L, U, I, J; "REAL" X;
  "ARRAY" A, B;
  "CODE" 34024;

  NORM:= 0;
  "FOR" I:= 1 "STEP" 1 "UNTIL" M "DO"
  "BEGIN" W:= 0;
    "FOR" J:= 1 "STEP" 1 "UNTIL" N "DO" W:= ABS(A[I,J]) + W;
    "IF" W > NORM "THEN" NORM:= W
  "END";
  MACHTOL:= EM[0] * NORM; EM[1]:= NORM;
  "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" I1:= I + 1; S:= TAMMAT(I1, M, I, I, A, A);
    "IF" S < MACHTOL "THEN" D[I]:= A[I,I] "ELSE"
    "BEGIN" F:= A[I,I]; S:= F * F + S;
      D[I]:= G:= "IF" F < 0 "THEN" SQRT(S) "ELSE" - SQRT(S);
      H:= F * G - S; A[I,I]:= F - G;
      "FOR" J:= I1 "STEP" 1 "UNTIL" N "DO"
      ELMCOL(I, M, J, I, A, A, TAMMAT(I, M, I, J, A, A) / H)
    "END";
    "IF" I < N "THEN"
    "BEGIN" S:= MATTAM(I1 + 1, N, I, I, A, A);
      "IF" S < MACHTOL "THEN" B[I]:= A[I,I1] "ELSE"
      "BEGIN" F:= A[I,I1]; S:= F * F + S;
        B[I]:= G:= "IF" F < 0 "THEN" SQRT(S) "ELSE" - SQRT(S);
        H:= F * G - S; A[I,I1]:= F - G;
        "FOR" J:= I1 "STEP" 1 "UNTIL" M "DO"
        ELMROW(I1, N, J, I, A, A, MATTAM(I1, N, I, J, A, A) /
        H)
      "END"
    "END"
  "END"
"END" HSHREABID;
"EOB"

```

```

"CODE" 34261;
"PROCEDURE" PSTTFMMAT(A, N, V, B);
"VALUE" N; "INTEGER" N; "ARRAY" A, V, B;
"BEGIN" "INTEGER" I, I1, J;
  "REAL" H;
  "REAL" "PROCEDURE" MATMAT(L, U, I, J, A, B);
  "VALUE" L, U, I, J; "INTEGER" L, U, I, J; "ARRAY" A, B;
  "CODE" 34013;
  "PROCEDURE" ELMCOL(L, U, I, J, A, B, X);
  "VALUE" L, U, I, J, X; "INTEGER" L, U, I, J; "REAL" X;
  "ARRAY" A, B;
  "CODE" 34023;

  I1:= N; V(N,N):= 1;
  "FOR" I:= N - 1 "STEP" - 1 "UNTIL" 1 "DO".
  "BEGIN" H:= B[I] * A[I,I1]; "IF" H < 0 "THEN"
    "BEGIN" "FOR" J:= I1 "STEP" 1 "UNTIL" N "DO" V[J,I]:= A[I,J] /
      H;
      "FOR" J:= I1 "STEP" 1 "UNTIL" N "DO"
        ELMCOL(I1, N, J, I, V, V, MATMAT(I1, N, I, J, A, V))
    "END";
    "FOR" J:= I1 "STEP" 1 "UNTIL" N "DO" V[I,J]:= V[J,I]:= 0;
    V[I,I]:= 1; I1:= I
  "END"
"END" PSTTFMMAT;
"EOP"

"CODE" 34262;
"PROCEDURE" PRETFMMAT(A, M, N, D);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, D;
"BEGIN" "INTEGER" I, I1, J;
  "REAL" G, H;
  "REAL" "PROCEDURE" TAMMAT(L, U, I, J, A, B);
  "VALUE" L, U, I, J; "INTEGER" L, U, I, J; "ARRAY" A, B;
  "CODE" 34014;
  "PROCEDURE" ELMCOL(L, U, I, J, A, B, X);
  "VALUE" L, U, I, J, X; "INTEGER" L, U, I, J; "REAL" X;
  "ARRAY" A, B;
  "CODE" 34023;

  "FOR" I:= N "STEP" - 1 "UNTIL" 1 "DO"
  "BEGIN" I1:= I + 1; G:= D[I]; H:= G * A[I,I];
    "FOR" J:= I1 "STEP" 1 "UNTIL" N "DO" A[I,J]:= 0;
    "IF" H < 0 "THEN"
      "BEGIN" "FOR" J:= I1 "STEP" 1 "UNTIL" N "DO"
        ELMCOL(I, M, J, I, A, A, TAMMAT(I1, M, I, J, A, A) / H);
        "FOR" J:= I "STEP" 1 "UNTIL" M "DO" A[J,I]:= A[J,I] / G
      "END"
    "ELSE"
      "FOR" J:= I "STEP" 1 "UNTIL" M "DO" A[J,I]:= 0;
      A[I,I]:= A[I,I] + 1
    "END"
  "END" PRETFMMAT;
"EOP"

```



SECTION 3.3.1.1.1

(JULY 1974)

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BRIEF DESCRIPTION:

THIS SECTION CONTAINS FOUR PROCEDURES FOR CALCULATING EIGENVALUES OR EIGENVECTORS OF A SYMMETRIC TRIDIAGONAL MATRIX.

VALSYMTRI CALCULATES ALL, OR SOME CONSECUTIVE, EIGENVALUES OF A SYMMETRIC TRIDIAGONAL MATRIX BY MEANS OF LINEAR INTERPOLATION USING A STURM SEQUENCE;

VECSYMTRI CALCULATES THE CORRESPONDING EIGENVECTORS BY MEANS OF INVERSE ITERATION.

QRVALSYMTRI CALCULATES ALL EIGENVALUES OF A SYMMETRIC TRIDIAGONAL MATRIX BY MEANS OF QR ITERATION;

QRISYMTRI CALCULATES THE EIGENVECTORS AS WELL.

WHEN ALL EIGENVALUES HAVE TO BE CALCULATED, QRVALSYMTRI IS PREFERABLE WITH RESPECT TO THE RUNNING TIME; WHEN THE EIGENVECTORS ALSO HAVE TO BE CALCULATED, INVERSE ITERATION IS PREFERABLE.

KEYWORDS:

EIGENVALUES,  
EIGENVECTORS,  
TRIDIAGONAL MATRIX,  
STURM-SEQUENCE,  
INVERSE ITERATION,  
QR ITERATION.

## SUBSECTION: VALSYMTRI.

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" VALSYMTRI(D, BB, N, N1, N2, VAL, EM);  
 "VALUE" N, N1, N2; "INTEGER" N, N1, N2;  
 "ARRAY" D, BB, VAL, EM;

## THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 D: <ARRAY IDENTIFIER>;  
 "ARRAY" D[1:N];  
 ENTRY: THE MAIN DIAGONAL OF THE SYMMETRIC TRIDIAGONAL  
 MATRIX;  
 BB: <ARRAY IDENTIFIER>;  
 "ARRAY" BB[1:N-1];  
 ENTRY: THE SQUARES OF THE CODIAGONAL ELEMENTS OF THE  
 SYMMETRIC TRIDIAGONAL MATRIX;  
 N1, N2: <ARITHMETIC EXPRESSION>;  
 THE SERIAL NUMBER OF THE FIRST AND LAST EIGENVALUE TO BE  
 CALCULATED, RESPECTIVELY;  
 VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[N1:N2];  
 EXIT: THE N2-N1+1 CALCULATED CONSECUTIVE EIGENVALUES IN  
 NONINCREASING ORDER;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:3];  
 ENTRY: EM[0], THE MACHINE PRECISION,  
 EM[1], AN UPPERBOUND FOR THE MODULI OF THE  
 EIGENVALUES OF THE GIVEN MATRIX,  
 EM[2], A RELATIVE TOLERANCE FOR THE EIGENVALUES;  
 EXIT: EM[3], THE TOTAL NUMBER OF ITERATIONS USED FOR  
 CALCULATING THE EIGENVALUES.

## PROCEDURES USED:

ZEROIN = CP34150.

## RUNNING TIME:

DEPENDS STRONGLY ON THE DISTANCE OF SUCCESSIVE EIGENVALUES.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

LET T DENOTE THE GIVEN SYMMETRIC TRIDIAGONAL MATRIX OF ORDER N AND I THE IDENTITY MATRIX. THE EIGENVALUES OF T ARE THE ZEROES OF THE N-TH DEGREE POLYNOMIAL  $P(N, X) = \det(T - X \cdot I)$ . INSTEAD OF SEARCHING FOR THE ZEROES OF  $P(N, X)$  WE LOOK FOR THE ZEROES OF THE FUNCTION  $F(N, X) = P(N, X) / P(N-1, X)$ . MAINTAINING A LOWER BOUND FOR  $\text{ABS}(P(N-1, X))$  WE DO AVOID OVERFLOW OF THE REAL NUMBER CAPACITY IN THE COMPUTATION OF  $F(N, X)$ . THIS FUNCTION CAN BE CALCULATED AS FOLLOWS:

```

F(1,X) = D[1] = X,
F(K,X) = D[K] = X + BB[K-1] /
("IF" ABS(F(K-1,X)) > MACHTOL "THEN" F(K-1,X)
"ELSE" "IF" F(K-1,X) <= 0 "THEN" =MACHTOL
"ELSE" MACHTOL), K = 2, . . . , N,

```

WHERE MACHTOL EQUALS  $EM[0] * EM[1]$ .

USING THE STURM SEQUENCE PROPERTY OF  $(F(K,X))$ ,  $K=1,2,\dots,N$ , WE CAN LOCATE THE DESIRED EIGENVALUES BY MEANS OF THE PROCEDURE ZEROIN (SECTION 5,1,1,1). FOR FURTHER DETAILS SEE REF[1], REF[2].

SUBSECTION: VEC SYM TRI.

CALLING SEQUENCE:

```

THE HEADING OF THE PROCEDURE IS:
"PROCEDURE" VEC SYM TRI(D, B, N, N1, N2, VAL, VEC, EM);
"VALUE" N, N1, N2; "INTEGER" N, N1, N2;
"ARRAY" D, B, VAL, VEC, EM;

```

THE MEANING OF THE FORMAL PARAMETERS IS:

```

N:      <ARITHMETIC EXPRESSION>;
        THE ORDER OF THE GIVEN MATRIX;
D:      <ARRAY IDENTIFIER>;
        "ARRAY" D[1:N];
        ENTRY: THE MAIN DIAGONAL OF THE SYMMETRIC TRIDIAGONAL
                MATRIX;
B:      <ARRAY IDENTIFIER>;
        "ARRAY" B[1:N];
        ENTRY: THE CODIAGONAL OF THE SYMMETRIC TRIDIAGONAL MATRIX
                FOLLOWED BY AN ADDITIONAL ELEMENT 0;
N1, N2: <ARITHMETIC EXPRESSION>;
        LOWER AND UPPER BOUND OF THE ARRAY VAL (SEE ALSO METHOD AND
        PERFORMANCE);
VAL:    <ARRAY IDENTIFIER>;
        "ARRAY" VAL[N1:N2];
        ENTRY: A ROW OF NONINCREASING EIGENVALUES AS DELIVERED BY
                VAL SYM TRI;
VEC:    <ARRAY IDENTIFIER>;
        "ARRAY" VEC[1:N,N1:N2];
        EXIT: THE EIGENVECTORS CORRESPONDING WITH THE GIVEN
                EIGENVALUES (SEE ALSO METHOD AND PERFORMANCE);
EM:     <ARRAY IDENTIFIER>;
        "ARRAY" EM[0:9];
        ENTRY: EM[0], THE MACHINE PRECISION,
                EM[1], A NORM OF THE GIVEN MATRIX,
                EM[4], THE ORTHOGONALISATION PARAMETER (SEE ALSO
                METHOD AND PERFORMANCE),
                EM[6], THE RELATIVE TOLERANCE FOR THE EIGENVECTORS,
                EM[8], THE MAXIMUM NUMBER OF ITERATIONS ALLOWED
                FOR THE CALCULATION OF EACH EIGENVECTOR;

```

EXIT: EM[5], THE NUMBER OF EIGENVECTORS INVOLVED IN THE  
 LAST GRAM-SCHMIDT ORTHOGONALISATION (SEE  
 METHOD AND PERFORMANCE),  
 EM[7], THE MAXIMUM EUCLIDEAN NORM OF THE RESIDUES,  
 EM[9], THE LARGEST NUMBER OF ITERATIONS PERFORMED  
 FOR THE CALCULATION OF SOME EIGENVECTOR (SEE  
 METHOD AND PERFORMANCE).

## PROCEDURES USED:

VECVEC = CP34010,  
 TAMVEC = CP34012,  
 ELMVECCOL = CP34021.

## REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: FIVE AUXILIARY ONE-DIMENSIONAL REAL ARRAYS  
 AND ONE BOOLEAN ARRAY, ALL OF LENGTH N, ARE USED.

RUNNING TIME: THE PROCESS IS OF ORDER N FOR EACH EIGENVECTOR.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

AN EIGENVECTOR OF A SYMMETRIC TRIDIAGONAL MATRIX T, CORRESPONDING  
 TO AN EIGENVALUE LAMBDA, IS CALCULATED BY MEANS OF INVERSE  
 ITERATION; I.E. STARTING FROM SOME INITIAL VECTOR X, THE LINEAR  
 SYSTEM  $(T - LAMBDA * I)Y = X$  IS SOLVED ITERATIVELY, THE SOLUTION Y,  
 DIVIDED BY ITS EUCLIDEAN NORM REPLACING X EACH TIME.  
 IF THE DISTANCE BETWEEN SOME APPROXIMATE EIGENVALUES IS SMALLER  
 THAN MACHTOL ( $=EM[0] * EM[1]$ ), THEN THEY ARE SLIGHTLY MODIFIED SUCH  
 THAT THE DISTANCE BETWEEN THEM EQUALS MACHTOL. IF THE DISTANCE  
 BETWEEN SOME EIGENVALUES IS SMALLER THAN THE ORTHOGONALISATION  
 PARAMETER ( $=EM[4]$ ) TIMES EM[1], THEN IN EACH ITERATION STEP GRAM-  
 SCHMIDT ORTHOGONALISATION IS CARRIED OUT, SO THAT THE EIGENVECTORS  
 OBTAINED ARE ORTHOGONAL WITHIN WORKING PRECISION. THE ITERATION  
 ENDS AS SOON AS EITHER THE EUCLIDEAN NORM OF THE RESIDUE IS SMALLER  
 THAN  $EM[1] * EM[6]$ , OR THE MAXIMUM ALLOWED NUMBER OF ITERATIONS  
 ( $=EM[8]$ ) HAS BEEN PERFORMED. IN THE LATTER CASE  $EM[9] := EM[8] + 1$ .  
 IF  $N1 > 1$ , THEN VEC SYMTRI SHOULD BE PRECEDED BY ONE OR MORE CALLS  
 OF VEC SYMTRI PRODUCING A NUMBER OF EIGENVECTORS CORRESPONDING TO  
 THE PRECEDING EIGENVALUES. MOREOVER ONE MUST GIVE EM[5], AS  
 PRODUCED BY THE LAST CALL OF VEC SYMTRI; THE K-TH TO N2-TH  
 EIGENVALUES, WHERE  $K = N1 - EM[5]$ , MUST BE GIVEN IN ARRAY VAL[K:N2]  
 IN MONOTONICALLY NONINCREASING ORDER (THE K-TH TO (N1-1)-TH  
 EIGENVALUES BEING NEEDED FOR THE MODIFYING MENTIONED ABOVE), AND  
 THE CORRESPONDING EIGENVECTORS UP TO THE (N1-1)-TH (WHICH ARE  
 NEEDED FOR THE GRAM-SCHMIDT ORTHOGONALISATION) IN THE CORRESPONDING  
 COLUMNS OF ARRAY VEC[1:N,K:N2].  
 THE TOLERANCES SHOULD SATISFY:  $EM[0] (< EM[2]) < EM[6]$  AND  
 $EM[4] >= EM[0] / EM[6]$ . FOR FURTHER DETAILS SEE REF[1].

SECTION 3.3.1.1.1

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SUBSECTION: QRIVALSYMTRI.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"INTEGER" "PROCEDURE" QRIVALSYMTRI (D, BB, N, EM);

"VALUE" N; "INTEGER" N; "ARRAY" D, BB, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: &lt;ARITHMETIC EXPRESSION&gt;;

THE ORDER OF THE GIVEN MATRIX;

D: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" D[1:N];

ENTRY: THE MAIN DIAGONAL OF THE SYMMETRIC TRIDIAGONAL MATRIX;

EXIT: THE EIGENVALUES OF THE MATRIX IN SOME ARBITRARY ORDER;

BB: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" BB[1:N];

ENTRY: THE SQUARES OF THE CODIAGONAL ELEMENTS OF THE SYMMETRIC TRIDIAGONAL MATRIX FOLLOWED BY AN ADDITIONAL ELEMENT 0;

EXIT: THE SQUARES OF THE CODIAGONAL ELEMENTS OF THE SYMMETRIC TRIDIAGONAL MATRIX RESULTING FROM THE QR ITERATION;

EM: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" EM[0:5];

ENTRY: EM[0], THE MACHINE PRECISION;

EM[1], A NORM OF THE GIVEN MATRIX;

EM[2], A RELATIVE TOLERANCE FOR THE EIGENVALUES;

EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;

EXIT: EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE CODIAGONAL ELEMENTS NEGLECTED;

EM[5], THE NUMBER OF ITERATIONS PERFORMED.

MOREOVER:

QRIVALSYMTRI: = THE NUMBER OF EIGENVALUES NOT CALCULATED.

PROCEDURES USED: NONE.

RUNNING TIME: THE PROCESS IS OF ORDER N SQUARED.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

IN QRIVALSYMTRI THE EIGENVALUES OF A SYMMETRIC TRIDIAGONAL MATRIX ARE CALCULATED BY MEANS OF QR-ITERATION. FOR THIS PROCEDURE WE USED ESSENTIALLY THE SQUARE-ROOT-FREE VERSION OF THE QR ALGORITHM DUE TO REINSCH[3].

IN ADDITION TO THE RELATIVE ERROR, WHICH IS SUPPOSED TO BE BOUNDED BY  $EM[1] * EM[2]$  (I.E. MATRIX NORM TIMES RELATIVE TOLERANCE), THE CALCULATED EIGENVALUES HAVE AN ABSOLUTE ERROR WHICH IS BOUNDED BY  $EM[0] * EM[1]$  (I.E. MACHINE PRECISION TIMES MATRIX NORM). IN PARTICULAR, WHEN SOME EIGENVALUES ARE VERY SMALL COMPARED TO THE MATRIX NORM, THE ACCURACY OF THE CALCULATED EIGENVALUES CAN BE INCREASED BY GIVING  $EM[0]$  A (POSITIVE) VALUE WHICH IS LESS THAN THE MACHINE PRECISION.

A PARTICULAR CHOICE OF  $EM[0]$  IS HARMLESS FOR THE PROCEDURE PROVIDED THAT FOR EACH I THE CALCULATION OF  $BB[I] / EM[0] ** 2$  CAUSES NO OVERFLOW AND THE CALCULATION OF  $(EM[0] * EM[1]) ** 2$  CAUSES NO UNDERFLOW.

ONE SHOULD NOTICE THAT THE NUMBER OF QR ITERATIONS INCREASES BY A SMALLER CHOICE OF  $EM[0]$ .

FOR FURTHER DETAILS SEE [2], [3].

## SUBSECTION: QRISYMTRI.

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"INTEGER" "PROCEDURE" QRISYMTRI(A, N, D, B, BB, EM);

"VALUE" N; "INTEGER" N; "ARRAY" A, D, B, BB, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;

THE ORDER OF THE GIVEN MATRIX;

D: <ARRAY IDENTIFIER>;

"ARRAY" D[1:N];

ENTRY: THE MAIN DIAGONAL OF THE SYMMETRIC TRIDIAGONAL MATRIX;

EXIT: THE EIGENVALUES OF THE MATRIX IN SOME ARBITRARY ORDER;

B: <ARRAY IDENTIFIER>;

"ARRAY" B[1:N];

ENTRY: THE CODIAGONAL OF THE SYMMETRIC TRIDIAGONAL MATRIX FOLLOWED BY AN ADDITIONAL ELEMENT 0;

EXIT: THE CODIAGONAL OF THE SYMMETRIC TRIDIAGONAL MATRIX RESULTING FROM THE QR ITERATION, FOLLOWED BY AN ADDITIONAL ELEMENT 0;

BB: <ARRAY IDENTIFIER>;

"ARRAY" BB[1:N];

ENTRY: THE SQUARED CODIAGONAL ELEMENTS OF THE SYMMETRIC TRIDIAGONAL MATRIX, FOLLOWED BY AN ADDITIONAL ELEMENT 0;

EXIT: THE SQUARED CODIAGONAL ELEMENTS OF THE SYMMETRIC TRIDIAGONAL MATRIX RESULTING FROM THE QR ITERATION;

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: SOME MATRIX S, SAY, (POSSIBLY THE IDENTITY MATRIX);  
 EXIT: THE EIGENVECTORS OF THE ORIGINAL SYMMETRIC  
 TRIDIAGONAL MATRIX, PREMULIPLIED BY S (SEE METHOD  
 AND PERFORMANCE);

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EM[1], A NORM OF THE GIVEN MATRIX;  
 EM[2], A RELATIVE TOLERANCE FOR THE QR ITERATION;  
 EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 EXIT: EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE CODIAGONAL  
 ELEMENTS NEGLECTED;  
 EM[5], THE NUMBER OF ITERATIONS PERFORMED,

MOREOVER;  
 GRISYMTRI:= THE NUMBER OF EIGENVALUES AND -VECTORS NOT  
 CALCULATED.

PROCEDURES USED:  
 ROTCOL = CP34040.

RUNNING TIME: . THE PROCESS IS OF ORDER N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

IN GRISYMTRI THE EIGENVALUES AND EIGENVECTORS OF A SYMMETRIC TRIDIAGONAL MATRIX ARE COMPUTED SIMULTANEOUSLY. IN MOST APPLICATIONS GRISYMTRI IS USED IN THE COMPUTATION OF EIGENVALUES AND -VECTORS OF A GENERAL SYMMETRIC MATRIX (SEE GRISYM SECTION 3.3.1.1.2); IN THAT CASE ARRAY A IS INITIALLY GIVEN THE VALUE OF THE TRANSFORMING MATRIX (TFMPREVEC SECTION 3.2.1.2.1.1). FOR THE COMPUTATION OF EIGENVALUES AND EIGENVECTORS OF A SYMMETRIC TRIDIAGONAL MATRIX, ARRAY A HAS TO BE INITIALIZED TO THE IDENTITY MATRIX. THE AVERAGE NUMBER OF ITERATIONS IS ABOUT 3N. WHEN THE PROCESS IS COMPLETED WITHIN EM[4] ITERATIONS, THEN GRISYMTRI:= 0; OTHERWISE GRISYMTRI:= THE NUMBER, K, OF EIGENVALUES NOT CALCULATED, EM[5]:= EM[4] + 1 AND ONLY THE LAST N - K ELEMENTS OF D AND THE LAST N - K COLUMNS OF A ARE APPROXIMATE EIGENVALUES AND -VECTORS RESPECTIVELY, OF THE ORIGINAL MATRIX. FOR FURTHER DETAILS SEE REF[1], REF[2].

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A STABLE, RATIONAL QR ALGORITHM FOR THE COMPUTATION OF THE  
EIGENVALUES OF AN HERMITIAN, TRIDIAGONAL MATRIX,  
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EXAMPLE OF USE:

THE FIRST AND SECOND EIGENVALUE IN MONOTONICALLY NON-INCREASING ORDER AND THE CORRESPONDING EIGENVECTORS OF T, WITH  $N = 4$  AND  $T[I,J] = \text{"IF" } I = J \text{ "THEN" } 2 \text{ "ELSE" "IF" } \text{ABS}(I - J) = 1 \text{ "THEN" } 1 \text{ "ELSE" } 0$ , MAY BE OBTAINED BY THE FOLLOWING PROGRAM:

```
"BEGIN"
  "INTEGER" J;
  "ARRAY" B, D[1:4], BB[1:3], VAL[1:2], EM[0:9], VEC[1:4,1:2];
  "PROCEDURE" VALSYMTRI(D, BB, N, N1, N2, VAL, EM); "CODE" 34151;
  "PROCEDURE" VECSYMTRI(D, B, N, N1, N2, VAL, VEC, EM); "CODE" 34152;

  EM[0] := "-14; EM[1] := 4; EM[2] := "-12;
  EM[4] := "-3; EM[6] := "-10; EM[8] := 5;
  "FOR" J := 1, 2, 3, 4 "DO" D[J] := 2; B[4] := 0;
  "FOR" J := 1, 2, 3 "DO"
  "BEGIN" BB[J] := 1; B[J] := -1 "END";
  VALSYMTRI(D, BB, 4, 1, 2, VAL, EM);
  VECSYMTRI(D, B, 4, 1, 2, VAL, VEC, EM);
  OUTPUT(61, "("2(+,13D"+2D, 2B), 2/)", VAL[1], VAL[2]);
  "FOR" J := 1, 2, 3, 4 "DO"
  OUTPUT(61, "("2(+,13D"+2D, 2B), /)", VEC[J,1], VEC[J,2]);
  OUTPUT(61, "("/, ,2D"+2D, /, 3(2ZD, /)",
  EM[7], EM[3], EM[5], EM[9])
"END"
```

THE PROGRAM DELIVERS:

THE EIGENVALUES: +,3618033988751"+01 +,2618033988750"+01

THE EIGENVECTORS: +,3717480344602"+00 +,6015009550075"+00  
 +,6015009550075"+00 +,3717480344602"+00  
 +,6015009550075"+00 -,3717480344602"+00  
 +,3717480344602"+00 -,6015009550075"+00

EM[7] = ,15"-11  
 EM[3] = 24  
 EM[5] = 1  
 EM[9] = 1 .



## SOURCE TEXT(S):

```

"CODE" 34151;
"COMMENT" MCA 2311;
"PROCEDURE" VALSYMTRI(D, BB, N, N1, N2, VAL, EM);
"VALUE" N, N1, N2;
"INTEGER" N, N1, N2; "ARRAY" D, BB, VAL, EM;
"BEGIN" "INTEGER" K, COUNT;
"REAL" MAX, X, Y, MACHEPS, NORM, RE, MACHTOL, UB, LB, LAMBDA;

"REAL" "PROCEDURE" STURM;
"BEGIN" "INTEGER" P, I; "REAL" F;
COUNT:= COUNT + 1;
P:= K; F:= D[I] = X;
"FOR" I:= 2 "STEP" 1 "UNTIL" N "DO"
"BEGIN" "IF" F <= 0 "THEN"
"BEGIN" P:= P + 1;
"IF" P > N "THEN" "GOTO" OUT
"END"
"ELSE" "IF" P < I - 1 "THEN"
"BEGIN" LB:= X; "GOTO" OUT "END";
"IF" ABS(F) < MACHTOL "THEN"
F:= "IF" F <= 0 "THEN" = MACHTOL "ELSE" MACHTOL;
F:= .D[I] = X = BB[I = 1] / F
"END";
"IF" P = N "OR" F <= 0 "THEN"
"BEGIN" "IF" X < UB "THEN" UB:= X "END" "ELSE" LB:= X;
OUT: STURM:= "IF" P = N "THEN" F "ELSE" (N = P) * MAX
"END" STURM;

"BOOLEAN" "PROCEDURE" ZEROIN(X, Y, FX, TOLX); "CODE" 34150;

MACHEPS:= EM[0]; NORM:= EM[1]; RE:= EM[2];
MACHTOL:= NORM * MACHEPS; MAX:= NORM / MACHEPS; COUNT:= 0;
UB:= 1,1 * NORM; LB:= = UB; LAMBDA:= UB;
"FOR" K:= N1 "STEP" 1 "UNTIL" N2 "DO"
"BEGIN" X:= LB; Y:= UB; LB:= =1,1 * NORM;
ZEROIN(X, Y, STURM, ABS(X) * RE + MACHTOL);
VAL[K]:= LAMBDA:= "IF" X > LAMBDA "THEN" LAMBDA "ELSE" X;
"IF" UB > X "THEN" UB:= "IF" X > Y "THEN" X "ELSE" Y
"END";
EM[3]:= COUNT
"END" VALSYMTRI;
"EOP"

```

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"CODE" 34152;
"COMMENT" MCA 2312;
"PROCEDURE" VECSYMTRI(D, B, N, N1, N2, VAL, VEC, EM);
"VALUE" N, N1, N2;
"INTEGER" N, N1, N2; "ARRAY" D, B, VAL, VEC, EM;
"BEGIN" "INTEGER" I, J, K, COUNT, MAXCOUNT, COUNTLIM, ORTH, IND;
"REAL" BI, BI1, U, W, Y, MI1, LAMBDA, OLDLAMBDA, ORTHEPS,
VALSPREAD, SPR, RES, MAXRES, OLDRES, NORM, NEWNORM, OLDNORM,
MACHTOL, VECTOL;
"ARRAY" M, P, Q, R, X[1:N];
"BOOLEAN" "ARRAY" INT[1:N];

"REAL" "PROCEDURE" VECVEC(L, U, SHIFT, A, B); "CODE" 34010;
"PROCEDURE" ELMVECCOL(L, U, I, A, B, X); "CODE" 34021;
"REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;

NORM:= EM[1]; MACHTOL:= EM[0] * NORM; VALSPREAD:= EM[4] * NORM;
VECTOL:= EM[6] * NORM; COUNTLIM:= EM[8]; ORTHEPS:= SQRT(EM[0]);
MAXCOUNT:= IND:= 0; MAXRES:= 0;
"IF" N1 > 1 "THEN"
"BEGIN" ORTH:= EM[5]; OLDLAMBDA:= VAL[N1 - ORTH];
"FOR" K:= N1 - ORTH + 1 "STEP" 1 "UNTIL" N1 - 1 "DO"
"BEGIN" LAMBDA:= VAL[K]; SPR:= OLDLAMBDA - LAMBDA;
"IF" SPR < MACHTOL "THEN" LAMBDA:= OLDLAMBDA - MACHTOL;
OLDLAMBDA:= LAMBDA
"END"
"END" "ELSE" ORTH:= 1;
"FOR" K:= N1 "STEP" 1 "UNTIL" N2 "DO"
"BEGIN" LAMBDA:= VAL[K]; "IF" K > 1 "THEN"
"BEGIN" SPR:= OLDLAMBDA - LAMBDA;
"IF" SPR < VALSPREAD "THEN"
"BEGIN" "IF" SPR < MACHTOL "THEN"
LAMBDA:= OLDLAMBDA - MACHTOL;
ORTH:= ORTH + 1
"END" "ELSE" ORTH:= 1
"END";
COUNT:= 0; U:= D[1] - LAMBDA; BI:= W:= B[1];
"IF" ABS(BI) < MACHTOL "THEN" BI:= MACHTOL;
"FOR" I:= 1 "STEP" 1 "UNTIL" N - 1 "DO"
"BEGIN" BI1:= BI + 1;
"IF" ABS(BI1) < MACHTOL "THEN" BI1:= MACHTOL;
"IF" ABS(BI) >= ABS(U) "THEN"
"BEGIN" MI1:= M[I + 1]:= U / BI; P[I]:= BI;
Y:= Q[I]:= D[I + 1] - LAMBDA; R[I]:= BI1;
U:= W - MI1 * Y; W:= - MI1 * BI1; INT[I]:= "TRUE"
"END"
"ELSE"
"BEGIN" MI1:= M[I + 1]:= BI / U; P[I]:= U; Q[I]:= W;
R[I]:= 0; U:= D[I + 1] - LAMBDA - MI1 * W; W:= BI1;
INT[I]:= "FALSE"
"END";
X[I]:= 1; BI:= BI1
"END" TRANSFORM

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P(N):= "IF" ABS(U) < MACHTOL "THEN" MACHTOL "ELSE" U;
Q(N):= R(N):= 0; X(N):= 1; "GOTO" ENTRY;
ITERATE: W:= X(1);
"FOR" I:= 2 "STEP" 1 "UNTIL" N "DO"
"BEGIN" "IF" INT(I = 1) "THEN"
"BEGIN" U:= W; W:= X(I - 1):= X(I) "END"
"ELSE" U:= X(I); W:= X(I):= U + M(I) * W
"END" ALTERNATE;
ENTRY: U:= W:= 0;
"FOR" I:= N "STEP" -1 "UNTIL" 1 "DO"
"BEGIN" Y:= U; U:= X(I):= (X(I) + Q(I) * U - R(I) * W) /
P(I); W:= Y
"END" NEXT ITERATION;
NEWNORM:= SQRT(VECVEC(1, N, 0, X, X)); "IF" ORTH > 1 "THEN"
"BEGIN" OLDNORM:= NEWNORM;
"FOR" J:= K + ORTH + 1 "STEP" 1 "UNTIL" K = 1 "DO"
ELMVECCOL(1, N, J, X, VEC, -TAMVEC(1, N, J, VEC, X));
NEWNORM:= SQRT(VECVEC(1, N, 0, X, X));
"IF" NEWNORM < ORTHEPS * OLDNORM "THEN"
"BEGIN" IND:= IND + 1; COUNT:= 1;
"FOR" I:= 1 "STEP" 1 "UNTIL" IND = 1,
IND + 1 "STEP" 1 "UNTIL" N "DO" X(I):= 0;
X(IND):= 1; "IF" IND = N "THEN" IND:= 0;
"GOTO" ITERATE
"END" NEW START
"END" ORTHOGONALISATION;
RES:= 1 / NEWNORM; "IF" RES > VECTOL "OR" COUNT = 0 "THEN"
"BEGIN" COUNT:= COUNT + 1; "IF" COUNT <= COUNTLIM "THEN"
"BEGIN" "FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
X(I):= X(I) * RES; "GOTO" ITERATE
"END"
"END";
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO" VEC(I,K):= X(I) * RES;
"IF" COUNT > MAXCOUNT "THEN" MAXCOUNT:= COUNT;
"IF" RES > MAXRES "THEN" MAXRES:= RES; OLDLAMBDA:= LAMBDA
"END";
EM(5):= ORTH; EM(7):= MAXRES; EM(9):= MAXCOUNT
"END" VEC SYMTRI;
"EQP"

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```

"CODE" 34160;
"INTEGER" "PROCEDURE" QRIVALSYMTRI(D, BB, N, EM); "VALUE" N;
"INTEGER" N; "ARRAY" D, BB, EM;
"BEGIN" "INTEGER" I, I1, LOW, OLDFLOW, N1, COUNT, MAX;
    "REAL" BBTOL, BBMAX, BBI, BBN1, MACHTOL, DN, DELTA, F, NUM,
    SHIFT, G, H, T, P, R, S, C, OLDFG;
    BBTOL:= (EM[2] * EM[1]) ** 2; MACHTOL:= EM[0] * EM[1];
    MAX:= EM[4]; BBMAX:= 0; COUNT:= 0; OLDFLOW:= N;
    "FOR" N1:= N - 1 "WHILE" N > 0 "DO"
    "BEGIN"
        "FOR" I:= N, I - 1 "WHILE" ("IF" I >= 1 "THEN"
        BB[I] > BBTOL "ELSE" "FALSE") "DO" LOW:= I;
        "IF" LOW > 1 "THEN" "BEGIN" "IF" BB[LOW-1] > BBMAX "THEN"
        BBMAX:= BB[LOW-1] "END";
        "IF" LOW = N "THEN" N1:= N1 "ELSE"
        "BEGIN" DN:= D[N]; DELTA:= D[N1] - DN;
            BBN1:= BB[N1];
            "IF" ABS(DELTA) < MACHTOL "THEN" R:= SQRT(BBN1) "ELSE"
            "BEGIN"
                F:= 2 / DELTA; NUM:= BBN1 * F;
                R:= -NUM / (SQRT(NUM * F + 1) + 1)
            "END";
            "IF" LOW = N1 "THEN"
            "BEGIN" D[N]:= DN + R; D[N1]:= D[N1] - R; N1:= N - 2
            "END"
            "ELSE"
            "BEGIN" COUNT:= COUNT + 1;
                "IF" COUNT > MAX "THEN" "GOTO" END;
                "IF" LOW < OLDFLOW "THEN"
                "BEGIN" SHIFT:= 0; OLDFLOW:= LOW "END"
                "ELSE" SHIFT:= DN + R;
                H:= D[LOW] - SHIFT;
                "IF" ABS(H) < MACHTOL "THEN" H:= "IF" H <= 0 "THEN"
                -MACHTOL "ELSE" MACHTOL;
                G:= H; T:= G * H;
                BBI:= BB[LOW]; P:= T + BBI; I1:= LOW;
                "FOR" I:= LOW + 1 "STEP" 1 "UNTIL" N "DO"
                "BEGIN" S:= BBI / P; C:= T / P;
                    H:= D[I] - SHIFT - BBI / H;
                    "IF" ABS(H) < MACHTOL "THEN" H:= "IF" H <= 0
                    "THEN" -MACHTOL "ELSE" MACHTOL;
                    OLDFG:= G; G:= H * C; T:= G * H;
                    D[I1]:= OLDFG - G + D[I];
                    BBI:= "IF" I = N "THEN" 0 "ELSE" BB[I];
                    P:= T + BBI; BB[I1]:= S * P; I1:= I
                "END";
                D[N]:= G + SHIFT
            "END" QRSTEP
        "END"
    "END"
"END";
END: EM[3]:= SQRT(BBMAX); EM[5]:= COUNT; QRIVALSYMTRI:= N
"END" QRIVALSYMTRI;
"EQP"
    
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"CODE" 34161;
"COMMENT" MCA 2321;
"INTEGER" "PROCEDURE" QRISYMTRI(A, N, D, B, BB, EM); "VALUE" N;
"INTEGER" N; "ARRAY" A, D, B, BB, EM;
"BEGIN" "INTEGER" I, J, J1, K, M, M1, COUNT, MAX;
      "REAL" BBMAX, R, S, SIN, T, C, COS, OLDCOS, G, P, W, TOL, TOL2,
      LAMBDA, DK1, A0, A1;

      "PROCEDURE" ROTCOL(L, U, I, J, A, C, S); "CODE" 34040;

      TOL:= EM[2] * EM[1]; TOL2:= TOL * TOL; COUNT:= 0; BBMAX:= 0;
      MAX:= EM[4]; M:= N;
      IN; K:= M; M1:= M - 1;
      NEXT: K:= K - 1; "IF" K > 0 "THEN"
        "BEGIN" "IF" BB[K] >= TOL2 "THEN" "GOTO" NEXT;
          "IF" BB[K] > BBMAX "THEN" BBMAX:= BB[K];
        "END";
        "IF" K = M1 "THEN" M:= M1 "ELSE"
          "BEGIN"
            T:= D[M] * D[M1]; R:= BB[M1];
            "IF" ABS(T) < TOL "THEN" S:= SQRT(R) "ELSE"
              "BEGIN" W:= 2 / T; S:= W * R / (SQRT(W * W * R + 1) + 1)
              "END"; "IF" K = M - 2 "THEN"
                "BEGIN" D[M]:= D[M] + S; D[M1]:= D[M1] * S;
                  T:= S / B[M1]; R:= SQRT(T * T + 1); COS:= 1 / R;
                  SIN:= T / R; ROTCOL(1, N, M1, M, A, COS, SIN); M:= M - 2
                "END"
              "ELSE"
                "BEGIN" COUNT:= COUNT + 1;
                  "IF" COUNT > MAX "THEN" "GOTO" END;
                  LAMBDA:= D[M] + S; "IF" ABS(T) < TOL "THEN"
                    "BEGIN" W:= D[M1] * S;
                      "IF" ABS(W) < ABS(LAMBDA) "THEN" LAMBDA:= W
                    "END";
                    K:= K + 1; T:= D[K] * LAMBDA; COS:= 1; W:= B[K];
                    P:= SQRT(T * T + W * W); J1:= K;
                    "FOR" J:= K + 1 "STEP" 1 "UNTIL" M "DO"
                      "BEGIN" OLDCOS:= COS; COS:= T / P; SIN:= W / P;
                        DK1:= D[J] * LAMBDA; T:= OLDCOS * T;
                        D[J1]:= (T + DK1) * SIN * SIN + LAMBDA * T;
                        T:= COS * DK1 * SIN * W * OLDCOS; W:= B[J];
                        P:= SQRT(T * T + W * W); G:= B[J1] * SIN * P;
                        BB[J1]:= G * G; ROTCOL(1, N, J1, J, A, COS, SIN);
                        J1:= J
                      "END";
                      D[M]:= COS * T + LAMBDA; "IF" T < 0 "THEN" B[M1]:= - G
                    "END" QRSTEP
                  "END";
                "IF" M > 0 "THEN" "GOTO" IN;
              END; EM[3]:= SQRT(BBMAX); EM[5]:= COUNT; QRISYMTRI:= M
            "END" QRISYMTRI;
          "EOP"

```

SECTION 3,3,1,1,2

(JULY 1974)

PAGE 1

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BRIEF DESCRIPTION:

THIS SECTION CONTAINS SEVEN PROCEDURES.  
 A) EIGVALSYM1 AND EIGVALSYM2 CALCULATE ALL EIGENVALUES, OR SOME CONSECUTIVE EIGENVALUES INCLUDING THE LARGEST, OF A SYMMETRIC MATRIX USING LINEAR INTERPOLATION ON A FUNCTION DERIVED FROM A STURM SEQUENCE,  
 B) EIGSYM1 AND EIGSYM2 CALCULATE THE CORRESPONDING EIGENVECTORS AS WELL, BY MEANS OF INVERSE ITERATION,  
 C) QRVALSYM1 AND QRVALSYM2 CALCULATE ALL EIGENVALUES OF A SYMMETRIC MATRIX BY MEANS OF QR ITERATION,  
 D) QRISYM CALCULATES ALL EIGENVECTORS AS WELL IN THE SAME ITERATION PROCESS.  
 EIGVALSYM1, EIGSYM1 AND QRVALSYM1 USE IONAL ARRAY FOR THE GIVEN SYMMETRIC MATRIX; THE OTHER PROCEDURES EXPECT THE MATRIX TO BE STORED IN "ARRAY".  
 QRISYM DELIVERS THE EIGENVECTORS IN THE ARRAY THAT WAS USED FOR THE ORIGINAL MATRIX IN CONTRAST WITH EIGSYM1 AND EIGSYM2 WHICH DELIVER THE EIGENVECTORS IN AN EXTRA ARRAY.  
 WHEN ALL EIGENVALUES HAVE TO BE CALCULATED, THE PROCEDURES USING QR ITERATION ARE PREFERABLE WITH RESPECT TO THEIR RUNNING TIME, WHEN ALSO THE EIGENVECTORS HAVE TO BE CALCULATED THE PROCEDURES USING INVERSE ITERATION ARE FASTER; HOWEVER, THE ONE USING QR ITERATION USES LESS MEMORY SPACE.

KEYWORDS:

EIGENVALUES,  
 EIGENVECTORS,  
 SYMMETRIC MATRIX,  
 STURM-SEQUENCE,  
 INVERSE ITERATION,  
 QR ITERATION.

SUBSECTION: EIGVALSYM2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" EIGVALSYM2(A, N, NUMVAL, VAL, EM);  
 "VALUE" N, NUMVAL; "INTEGER" N, NUMVAL; "ARRAY" A, VAL, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 NUMVAL: <ARITHMETIC EXPRESSION>;  
 THE SERIAL NUMBER OF THE LAST EIGENVALUE TO BE CALCULATED;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE UPPER TRIANGLE OF THE SYMMETRIC MATRIX MUST BE  
 GIVEN IN THE UPPER TRIANGULAR PART OF A (THE  
 ELEMENTS A[I,J], I ≤ J);  
 EXIT: THE DATA FOR HOUSEHOLDER'S BACK TRANSFORMATION  
 (WHICH ISN'T USED BY THIS PROCEDURE) IS DELIVERED  
 IN THE UPPER TRIANGULAR PART OF A;  
 THE ELEMENTS A[I,J] FOR I > J ARE NEITHER USED NOR CHANGED;  
 VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:NUMVAL];  
 EXIT: THE NUMVAL LARGEST EIGENVALUES IN MONOTONICALLY  
 NON-INCREASING ORDER;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:3];  
 ENTRY: EM[0], THE MACHINE PRECISION,  
 EM[2], THE RELATIVE TOLERANCE FOR THE EIGENVALUES;  
 EXIT: EM[1], THE INFINITY NORM OF THE ORIGINAL MATRIX,  
 EM[3], THE NUMBER OF ITERATIONS USED FOR  
 CALCULATING THE NUMVAL EIGENVALUES.

PROCEDURES USED:

TFMSYMTRI2 = CP34140,  
 VALSYMTRI = CP34151.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:

THREE ONE-DIMENSIONAL REAL ARRAYS OF LENGTH N ARE USED.

RUNNING TIME:

ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE BODY OF EIGVALSYM2 CONSISTS OF TWO PROCEDURE STATEMENTS; THE  
 FIRST IS A CALL OF TFMSYMTRI2 TO TRANSFORM THE SYMMETRIC MATRIX  
 INTO A SIMILAR TRIDIAGONAL MATRIX BY MEANS OF HOUSEHOLDER'S  
 TRANSFORMATION; THE SECOND IS A CALL OF VALSYMTRI TO CALCULATE THE  
 DESIRED EIGENVALUES. OPERATION DETAILS OF BOTH PROCEDURES ARE GIVEN  
 IN THEIR DESCRIPTION.

SUBSECTION: EIGVALSYM1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" EIGVALSYM1(A, N, NUMVAL, VAL, EM);  
 "VALUE" N, NUMVAL; "INTEGER" N, NUMVAL; "ARRAY" A, VAL, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 NUMVAL: <ARITHMETIC EXPRESSION>;  
 THE SERIAL NUMBER OF THE LAST EIGENVALUE TO BE CALCULATED;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:(N+1)\*N//2];  
 ENTRY: THE UPPER TRIANGLE OF THE SYMMETRIC MATRIX MUST BE  
 GIVEN IN SUCH A WAY THAT THE (I,J)-TH ELEMENT OF  
 THE MATRIX IS A[(J-1)\*J//2+I],  $1 \leq I \leq J \leq N$ ;  
 EXIT: THE DATA FOR HOUSEHOLDER'S BACK TRANSFORMATION  
 (WHICH ISN'T USED BY THIS PROCEDURE).  
 VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:NUMVAL];  
 EXIT: THE NUMVAL LARGEST EIGENVALUES IN MONOTONICALLY  
 NON-INCREASING ORDER;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:3];  
 ENTRY: EM[0], THE MACHINE PRECISION,  
 EM[2], THE RELATIVE TOLERANCE FOR THE EIGENVALUES;  
 EXIT: EM[1], THE INFINITY NORM OF THE ORIGINAL MATRIX,  
 EM[3], THE NUMBER OF ITERATIONS USED FOR  
 CALCULATING THE NUMVAL EIGENVALUES.

PROCEDURES USED:

TFMSYMTRI1 = CP34143,  
 VALSYMTRI = CP34151.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:

THREE ONE-DIMENSIONAL REAL ARRAYS OF LENGTH N ARE USED.

RUNNING TIME:

ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE BODY OF EIGVALSYM1 CONSISTS OF TWO PROCEDURE STATEMENTS; THE FIRST IS A CALL OF TFMSYMTRI1 TO TRANSFORM THE SYMMETRIC MATRIX INTO A SIMILAR TRIDIAGONAL MATRIX BY MEANS OF HOUSEHOLDER'S TRANSFORMATION; THE SECOND IS A CALL OF VALSYMTRI TO CALCULATE THE DESIRED EIGENVALUES. OPERATION DETAILS OF BOTH PROCEDURES ARE GIVEN IN THEIR DESCRIPTION.



SUBSECTION: EIGSYM2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"PROCEDURE" EIGSYM2(A, N, NUMVAL, VAL, VEC, EM);

"VALUE" N, NUMVAL; "INTEGER" N, NUMVAL; "ARRAY" A, VAL, VEC, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;

THE ORDER OF THE GIVEN MATRIX;

NUMVAL: <ARITHMETIC EXPRESSION>;

THE SERIAL NUMBER OF THE LAST EIGENVALUE TO BE CALCULATED;

A: <ARRAY IDENTIFIER>;

"ARRAY" A[1:N,1:N];

ENTRY: THE UPPER TRIANGLE OF THE SYMMETRIC MATRIX MUST BE GIVEN IN THE UPPER TRIANGULAR PART OF A (THE ELEMENTS A[I,J], I ≤ J);

EXIT: THE DATA FOR HOUSEHOLDER'S BACK TRANSFORMATION IS DELIVERED IN THE UPPER TRIANGULAR PART OF A;

THE ELEMENTS A[I,J] FOR I > J ARE NEITHER USED NOR CHANGED;

VAL: <ARRAY IDENTIFIER>;

"ARRAY" VAL[1:NUMVAL];

EXIT: THE NUMVAL LARGEST EIGENVALUES IN MONOTONICALLY NON-INCREASING ORDER;

VEC: <ARRAY IDENTIFIER>;

"ARRAY" VEC[1:N,1:NUMVAL];

EXIT: THE NUMVAL CALCULATED EIGENVECTORS, STORED COLUMNWISE, CORRESPONDING TO THE CALCULATED EIGENVALUES;

EM: <ARRAY IDENTIFIER>;

"ARRAY" EM[0:9];

ENTRY: EM[0], THE MACHINE PRECISION,  
EM[2], THE RELATIVE TOLERANCE FOR THE EIGENVALUES,  
EM[4], THE ORTHOGONALISATION PARAMETER (SEE METHOD AND PERFORMANCE),

EM[6], THE TOLERANCE FOR THE EIGENVECTORS,

EM[8], THE MAXIMUM NUMBER OF INVERSE ITERATIONS ALLOWED FOR THE CALCULATION OF EACH EIGENVECTOR;

EXIT: EM[1], THE INFINITY NORM OF THE MATRIX,

EM[3], THE NUMBER OF ITERATIONS USED FOR CALCULATING THE NUMVAL EIGENVALUES,

EM[5], THE NUMBER OF EIGENVECTORS INVOLVED IN THE LAST GRAM-SCHMIDT ORTHOGONALISATION,

EM[7], THE MAXIMUM EUCLIDEAN NORM OF THE RESIDUES OF THE CALCULATED EIGENVECTORS,

EM[9], THE LARGEST NUMBER OF INVERSE ITERATIONS PERFORMED FOR THE CALCULATION OF SOME EIGENVECTOR.

PROCEDURES USED:

TFMSYMTR12	=	CP34140,
VALSYMTRI	=	CP34151,
VECSYMTRI	=	CP34152,
BAKSYMTR12	=	CP34141.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:

THREE ONE-DIMENSIONAL REAL ARRAYS OF LENGTH N ARE DECLARED;  
 MOREOVER, VECSYMTRI USES FIVE ONE-DIMENSIONAL REAL ARRAYS  
 OF LENGTH N AND ONE BOOLEAN ARRAY OF LENGTH N.

RUNNING TIME:

ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE BODY OF EIGSYM2 CONSISTS OF FOUR PROCEDURE STATEMENTS;  
 THE FIRST IS A CALL OF TFMSYMTR12 TO TRANSFORM THE SYMMETRIC  
 MATRIX INTO A SIMILAR TRIDIAGONAL MATRIX BY MEANS OF  
 HOUSEHOLDERS TRANSFORMATION,  
 THE SECOND IS A CALL OF VALSYMTRI TO CALCULATE THE DESIRED  
 EIGENVALUES,  
 THE THIRD IS A CALL OF VECSYMTRI TO CALCULATE THE CORRESPONDING  
 EIGENVECTORS AND  
 THE FOURTH IS A CALL OF BAKSYMTR12 TO PERFORM THE BACK  
 TRANSFORMATION.  
 THE PARAMETERS EM[5], EM[7] AND EM[9] ARE GIVEN ITS VALUE IN THE  
 PROCEDURE VECSYMTRI. FOR A POSSIBLY SUBSEQUENT CALL OF VECSYMTRI  
 THE VALUE OF EM[5] IS NEEDED. WHEN CONSECUTIVE EIGENVALUES ARE TOO  
 CLOSE TOGETHER, THE CORRESPONDING EIGENVECTORS ARE NOT NECESSARILY  
 DELIVERED ORTHOGONAL BY INVERSE ITERATION (THE METHOD WHICH IS USED  
 IN VECSYMTRI). THEREFORE GRAM-SCHMIDT ORTHOGONALISATION IS APPLIED  
 ON THE EIGENVECTORS WHEN THE DISTANCE BETWEEN TWO CONSECUTIVE  
 EIGENVALUES IS SMALLER THAN EM[4].  
 FOR FURTHER DETAILS ONE IS REFERRED TO THE SPECIFIC PROCEDURE  
 DESCRIPTIONS.

SUBSECTION: EIGSYM1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" EIGSYM1(A, N, NUMVAL, VAL, VEC, EM);  
 "VALUE" N, NUMVAL; "INTEGER" N, NUMVAL; "ARRAY" A, VAL, VEC, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 NUMVAL: <ARITHMETIC EXPRESSION>;  
 THE SERIAL NUMBER OF THE LAST EIGENVALUE TO BE CALCULATED;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:(N+1)\*N//2];  
 ENTRY: THE UPPER TRIANGLE OF THE SYMMETRIC MATRIX MUST BE  
 GIVEN IN SUCH A WAY THAT THE (I,J)-TH ELEMENT OF  
 THE MATRIX IS A[(J-1)\*J//2+I], 1 <= I <= J <= N;  
 EXIT: THE DATA FOR HOUSEHOLDER'S BACK TRANSFORMATION;  
 VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:NUMVAL];  
 EXIT: THE NUMVAL LARGEST EIGENVALUES IN MONOTONICALLY  
 NON-INCREASING ORDER;  
 VEC: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC[1:N,1:NUMVAL];  
 EXIT: THE NUMVAL CALCULATED EIGENVECTORS, STORED COLUMN-  
 WISE, CORRESPONDING TO THE CALCULATED EIGENVALUES;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:9];  
 ENTRY: EM[0], THE MACHINE PRECISION,  
 EM[2], THE RELATIVE TOLERANCE FOR THE EIGENVALUES,  
 EM[4], THE ORTHOGONALISATION PARAMETER (SEE METHOD  
 AND PERFORMANCE),  
 EM[6], THE TOLERANCE FOR THE EIGENVECTORS,  
 EM[8], THE MAXIMUM NUMBER OF INVERSE ITERATIONS  
 ALLOWED FOR THE CALCULATION OF EACH EIGEN-  
 VECTOR;  
 EXIT: EM[1], THE INFINITY NORM OF THE MATRIX,  
 EM[3], THE NUMBER OF ITERATIONS USED FOR  
 CALCULATING THE NUMVAL EIGENVALUES,  
 EM[5], THE NUMBER OF EIGENVECTORS INVOLVED IN THE  
 LAST GRAM-SCHMIDT ORTHOGONALISATION,  
 EM[7], THE MAXIMUM EUCLIDEAN NORM OF THE RESIDUES  
 OF THE CALCULATED EIGENVECTORS,  
 EM[9], THE LARGEST NUMBER OF INVERSE ITERATIONS  
 PERFORMED FOR THE CALCULATION OF SOME EIGEN-  
 VECTOR.

## PROCEDURES USED:

TFMSYMTRI1	=	CP34143,
VALSYMTRI	=	CP34151,
VECSYMTRI	=	CP34152,
BAKSYMTRI1	=	CP34144.

## REQUIRED CENTRAL MEMORY:

## EXECUTION FIELD LENGTH:

THREE ONE-DIMENSIONAL REAL ARRAYS OF LENGTH N ARE DECLARED;  
MOREOVER, VECASYMTRI AND BAKSYMTRI1 USE A TOTAL AMOUNT OF  
SIX ONE-DIMENSIONAL REAL ARRAYS OF LENGTH N AND ONE BOOLEAN  
ARRAY OF LENGTH N.

## RUNNING TIME:

ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

THE BODY OF EIGSYM1 CONSISTS OF FOUR PROCEDURE STATEMENTS;  
THE FIRST IS A CALL OF TFMSYMTRI1 TO TRANSFORM THE SYMMETRIC  
MATRIX INTO A SIMILAR TRIDIAGONAL MATRIX BY MEANS OF  
HOUSEHOLDERS TRANSFORMATION,  
THE SECOND IS A CALL OF VALSYMTRI TO CALCULATE THE DESIRED  
EIGENVALUES,  
THE THIRD IS A CALL OF VECASYMTRI TO CALCULATE THE CORRESPONDING  
EIGENVECTORS AND  
THE FOURTH IS A CALL OF BAKSYMTRI1 TO PERFORM THE BACK  
TRANSFORMATION.  
FOR DETAILS ONE IS REFERRED TO EIGSYM2 OR TO THE DESCRIPTIONS OF  
THE FOUR PROCEDURES USED.

SUBSECTION: QRIVALSYM2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "INTEGER" "PROCEDURE" QRIVALSYM2(A, N, VAL, EM);  
 "VALUE" N; "INTEGER" N; "ARRAY" A, VAL, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE UPPER TRIANGLE OF THE SYMMETRIC MATRIX MUST BE  
 GIVEN IN THE UPPER TRIANGULAR PART OF A (THE  
 ELEMENTS A[I,J], I<= J);  
 EXIT: THE DATA FOR HOUSEHOLDER'S BACK TRANSFORMATION  
 (WHICH ISN'T USED BY THIS PROCEDURE) IS DELIVERED  
 IN THE UPPER TRIANGULAR PART OF A;  
 THE ELEMENTS A[I,J] FOR I > J ARE NEITHER USED NOR CHANGED;  
 VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:N];  
 EXIT: THE EIGENVALUES OF THE MATRIX IN SOME ARBITRARY  
 ORDER;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0], THE MACHINE PRECISION,  
 EM[2], THE RELATIVE TOLERANCE FOR THE EIGENVALUES,  
 EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 EXIT: EM[1], THE INFINITY NORM OF THE MATRIX,  
 EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE CODIAGONAL  
 ELEMENTS NEGLECTED,  
 EM[5], THE NUMBER OF ITERATIONS PERFORMED;

MOREOVER:  
 QRIVALSYM2 := THE NUMBER OF EIGENVALUES NOT CALCULATED.

PROCEDURES USED:

TFMSYMTRI2 = CP34140,  
 QRIVALSYMTRI = CP34160.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:  
 IONAL REAL ARRAYS OF LENGTH N ARE USED.

RUNNING TIME:

ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE BODY OF QRIVALSYM2 CONSISTS OF TWO PROCEDURE STATEMENTS; THE FIRST IS A CALL OF TFMSYMTRI2 TO TRANSFORM THE SYMMETRIC MATRIX INTO A SIMILAR TRIDIAGONAL MATRIX BY MEANS OF HOUSEHOLDER'S TRANSFORMATION; THE SECOND IS A CALL OF QRIVALSYMTRI TO CALCULATE THE EIGENVALUES. WHEN THE PROCESS IS COMPLETED WITHIN EM[4] ITERATIONS THEN QRIVALSYM2:= 0; OTHERWISE QRIVALSYM2:= THE NUMBER, K, OF EIGENVALUES NOT CALCULATED, EM[5]:= EM[4] + 1 AND ONLY THE LAST N - K ELEMENTS OF VAL ARE APPROXIMATE EIGENVALUES OF THE GIVEN MATRIX. OPERATION DETAILS OF BOTH PROCEDURES USED ARE GIVEN IN THEIR DESCRIPTION.

SUBSECTION: QRIVALSYM1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "INTEGER" "PROCEDURE" QRIVALSYM1(A, N, VAL, EM);  
 "VALUE" N; "INTEGER" N; "ARRAY" A, VAL, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:(N+1)\*N//2];  
 ENTRY: THE UPPER TRIANGLE OF THE SYMMETRIC MATRIX MUST BE GIVEN IN SUCH A WAY THAT THE (I,J)-TH ELEMENT OF THE MATRIX IS A[(J-1)\*J//2+I], 1 <= I <= J <= N;  
 EXIT: THE DATA FOR HOUSEHOLDER'S BACK TRANSFORMATION (WHICH ISN'T USED BY THIS PROCEDURE).  
 VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:N];  
 EXIT: THE EIGENVALUES OF THE MATRIX IN SOME ARBITRARY ORDER;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0], THE MACHINE PRECISION,  
 EM[2], THE RELATIVE TOLERANCE FOR THE EIGENVALUES,  
 EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 EXIT: EM[1], THE INFINITY NORM OF THE MATRIX,  
 EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE CODIAGONAL ELEMENTS NEGLECTED,  
 EM[5], THE NUMBER OF ITERATIONS PERFORMED;

MOREOVER:

QRIVALSYM1:= THE NUMBER OF EIGENVALUES NOT CALCULATED.

PROCEDURES USED:

TFMSYMTRI1 = CP34143,  
 QRIVALSYMTRI = CP34160.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:

TWO ONE-DIMENSIONAL REAL ARRAYS OF LENGTH N ARE USED.

RUNNING TIME:  
ROUGHLY PROPORTIONAL TO N CUBED,

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE BODY OF QRVALSYM1 CONSISTS OF TWO PROCEDURE STATEMENTS; THE FIRST IS A CALL OF TFMSYMTRI1 TO TRANSFORM THE SYMMETRIC MATRIX INTO A SIMILAR TRIDIAGONAL MATRIX BY MEANS OF HOUSEHOLDER'S TRANSFORMATION; THE SECOND IS A CALL OF QRVALSYMTRI TO CALCULATE THE EIGENVALUES. WHEN THE PROCESS IS COMPLETED WITHIN EM[4] ITERATIONS THEN QRVALSYM1:= 0; OTHERWISE QRVALSYM1:= THE NUMBER, K, OF EIGENVALUES NOT CALCULATED, EM[5]:= EM[4] + 1 AND ONLY THE LAST N - K ELEMENTS OF VAL ARE APPROXIMATE EIGENVALUES OF THE GIVEN MATRIX. OPERATION DETAILS OF BOTH PROCEDURES USED ARE GIVEN IN THEIR DESCRIPTION.

SUBSECTION: QRISYM.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
"INTEGER" "PROCEDURE" QRISYM(A, N, VAL, EM);  
"VALUE" N; "INTEGER" N; "ARRAY" A, VAL, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE GIVEN MATRIX;  
A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1:N,1:N];  
ENTRY: THE UPPER TRIANGLE OF THE SYMMETRIC MATRIX MUST BE GIVEN IN THE UPPER TRIANGULAR PART OF A (THE ELEMENTS A[I,J], I<= J);  
EXIT: THE EIGENVECTORS OF THE SYMMETRIC MATRIX, STORED COLUMNWISE;  
VAL: <ARRAY IDENTIFIER>;  
"ARRAY" VAL[1:N];  
EXIT: THE EIGENVALUES OF THE MATRIX CORRESPONDING TO THE CALCULATED EIGENVECTORS;  
EM: <ARRAY IDENTIFIER>;  
"ARRAY" EM[0:5];  
ENTRY: EM[0], THE MACHINE PRECISION,  
EM[2], THE RELATIVE TOLERANCE FOR THE QR ITERATION,  
EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
EXIT: EM[1], THE INFINITY NORM OF THE MATRIX,  
EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE CODIAGONAL ELEMENTS NEGLECTED,  
EM[5], THE NUMBER OF ITERATIONS PERFORMED;

MOREOVER:

QRISYM := THE NUMBER OF EIGENVALUES AND -VECTORS NOT CALCULATED.

PROCEDURES USED:

TFMSYMTRI2        =       CP34140,  
TFMPREVEC         =       CP34142,  
QRISYMTRI         =       CP34161.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:

TWO ONE-DIMENSIONAL REAL ARRAYS OF LENGTH N ARE USED.

RUNNING TIME:

PROPORTIONAL TO N CUBED.

LANGUAGE:    ALGOL 60.

METHOD AND PERFORMANCE:

THE BODY OF QRISYM CONSISTS OF THREE PROCEDURE STATEMENTS; THE FIRST IS A CALL OF TFMSYMTRI2 TO TRANSFORM THE SYMMETRIC MATRIX INTO A SIMILAR TRIDIAGONAL MATRIX BY MEANS OF HOUSEHOLDER'S TRANSFORMATION, THE SECOND IS A CALL OF TFMPREVEC TO PERFORM THE DESIRED BACK TRANSFORMATION ON THE EIGENVECTORS IN ADVANCE AND THE THIRD IS A CALL OF QRISYMTRI TO CALCULATE THE EIGENVALUES AND THE EIGENVECTORS. WHEN THE PROCESS IS COMPLETED WITHIN EM[4] ITERATIONS THEN QRISYM:= 0; OTHERWISE QRISYM:= THE NUMBER, K, OF EIGENVALUES AND VECTORS NOT CALCULATED, EM[5]:= EM[4] + 1 AND ONLY THE LAST N - K ELEMENTS OF VAL AND THE LAST N - K COLUMNS OF A ARE APPROXIMATE EIGENVALUES AND EIGENVECTORS RESPECTIVELY OF THE GIVEN MATRIX. OPERATION DETAILS OF THE PROCEDURES USED ARE GIVEN IN THEIR DESCRIPTION.

EXAMPLES OF USE:

THE TWO LARGEST EIGENVALUES IN MONOTONICALLY NON INCREASING ORDER AND THE CORRESPONDING EIGENVECTORS OF M, WITH N = 4 AND  $M[I,J] = 1 / (I + J - 1)$ , MAY BE OBTAINED BY THE FOLLOWING PROGRAM:

```
"BEGIN"
  "INTEGER" I, J;
  "ARRAY" A[1:10], VAL[1:2], EM[0:9], VEC[1:4,1:2];
  "PROCEDURE" EIGSYM1(A, N, NUMVAL, VAL, VEC, EM); "CODE" 34156;

  EM[0]:= "-14; EM[2]:= "-12; EM[4]:= "-3;
  EM[6]:= 10"-10; EM[8]:= 5;
  "FOR" I:= 1 "STEP" 1 "UNTIL" 4 "DO"
  "FOR" J:= I "STEP" 1 "UNTIL" 4 "DO"
  A[(J * J - J) / 2 + I]:= 1 / (I + J - 1);
  EIGSYM1(A, 4, 2, VAL, VEC, EM);
  OUTPUT(61, "(2(+.13D"+2D, 2B), 2/)", VAL[1], VAL[2]);
  "FOR" I:= 1, 2, 3, 4 "DO"
  OUTPUT(61, "(2(+.13D"+2D, 2B), /)", VEC[I,1], VEC[I,2]);
  OUTPUT(61, "(2(.2D"+2D, /), 3(2ZD, /)",
  EM[1], EM[7], EM[3], EM[5], EM[9])
"END"
```



THE PROGRAM DELIVERS (THE RESULTS ARE CORRECT UP TO TWELVE DIGITS):

THE EIGENVALUES: +.1500214280059"+01 +.1691412202214"+00

THE EIGENVECTORS: -.7926082911638"+00 +.5820756994972"+00  
 =.4519231209016"+00 =.3705021850671"+00  
 =.3224163985818"+00 =.5095786345018"+00  
 =.2521611696882"+00 =.5140482722222"+00

EM[1] = .21"+01  
 EM[7] = .92"-14  
 EM[3] = 32  
 EM[5] = 1  
 EM[9] = 1 .

THE TWO LARGEST EIGENVALUES OF M, WITH N = 4 AND M[I,J] = 1 / (I + J - 1), MAY BE OBTAINED IN MONOTONICALLY NON INCREASING ORDER BY THE FOLLOWING PROGRAM:

```
"BEGIN"
  "INTEGER" I, J
  "ARRAY" A[1:4,1:4], VAL[1:2], EM[0:3];
  "PROCEDURE" EIGVALSYM2(A, N, NUMVAL, VAL, EM); "CODE" 34153;

  EM[0] := "-14; EM[2] := "-12;
  "FOR" I := 1 "STEP" 1 "UNTIL" 4 "DO"
  "FOR" J := I "STEP" 1 "UNTIL" 4 "DO" A[I,J] := 1 / (I + J - 1);
  EIGVALSYM2(A, 4, 2, VAL, EM);
  OUTPUT(61, "("2(+.13D"+2D, 2B)"); VAL[1], VAL[2]);
  OUTPUT(61, "("2/, .2D"+2D, /, 2ZD)"; EM[1], EM[3])
"END"
```

THE PROGRAM DELIVERS (THE RESULTS ARE CORRECT UP TO TWELVE DIGITS):

THE EIGENVALUES: +.1500214280059"+01 +.1691412202214"+00  
 EM[3] = .21"+01  
 EM[1] = 32 .

SOURCE TEXT(S) :

```

"CODE" 34153;
"COMMENT" MCA 2313;
"PROCEDURE" EIGVALSYM2(A, N, NUMVAL, VAL, EM); "VALUE" N, NUMVAL;
"INTEGER" N, NUMVAL; "ARRAY" A, VAL, EM;
"BEGIN" "ARRAY" B, BB, D[1:N];

      "PROCEDURE" TFMSYMTRI2(A, N, D, B, BB, EM); "CODE" 34140;
      "PROCEDURE" VALSYMTRI(D, BB, N, N1, N2, VAL, EM); "CODE" 34151;

      TFMSYMTRI2(A, N, D, B, BB, EM);
      VALSYMTRI(D, BB, N, 1, NUMVAL, VAL, EM)
"END" EIGVALSYM2;
"EOP"

"CODE" 34154;
"COMMENT" MCA 2314;
"PROCEDURE" EIGSYM2(A, N, NUMVAL, VAL, VEC, EM); "VALUE" N, NUMVAL;
"INTEGER" N, NUMVAL; "ARRAY" A, VAL, VEC, EM;
"BEGIN" "ARRAY" B, BB, D[1:N];

      "PROCEDURE" TFMSYMTRI2(A, N, D, B, BB, EM); "CODE" 34140;
      "PROCEDURE" VALSYMTRI(D, BB, N, N1, N2, VAL, EM); "CODE" 34151;
      "PROCEDURE" VECSYMTRI(D, B, N, N1, N2, VAL, VEC, EM);
      "CODE" 34152;
      "PROCEDURE" BAKSYMTRI2(A, N, N1, N2, VEC); "CODE" 34141;

      TFMSYMTRI2(A, N, D, B, BB, EM);
      VALSYMTRI(D, BB, N, 1, NUMVAL, VAL, EM);
      VECSYMTRI(D, B, N, 1, NUMVAL, VAL, VEC, EM);
      BAKSYMTRI2(A, N, 1, NUMVAL, VEC)
"END" EIGSYM2;
"EOP"

"CODE" 34155;
"COMMENT" MCA 2318;
"PROCEDURE" EIGVALSYM1(A, N, NUMVAL, VAL, EM); "VALUE" N, NUMVAL;
"INTEGER" N, NUMVAL; "ARRAY" A, VAL, EM;
"BEGIN" "ARRAY" B, BB, D[1:N];

      "PROCEDURE" TFMSYMTRI1(A, N, D, B, BB, EM); "CODE" 34143;
      "PROCEDURE" VALSYMTRI(D, BB, N, N1, N2, VAL, EM); "CODE" 34151;

      TFMSYMTRI1(A, N, D, B, BB, EM);
      VALSYMTRI(D, BB, N, 1, NUMVAL, VAL, EM)
"END" EIGVALSYM1;
"EOP"

```

```

"CODE" 34156;
"COMMENT" MCA 2319;
"PROCEDURE" EIGSYM1(A, N, NUMVAL, VAL, VEC, EM); "VALUE" N, NUMVAL;
"INTEGER" N, NUMVAL; "ARRAY" A, VAL, VEC, EM;
"BEGIN" "ARRAY" B, BB, D[1:N];

      "PROCEDURE" TFMSYMTRI1(A, N, D, B, BB, EM); "CODE" 34143;
      "PROCEDURE" VALSYMTRI(D, BB, N, N1, N2, VAL, EM); "CODE" 34151;
      "PROCEDURE" VECSYMTRI(D, B, N, N1, N2, VAL, VEC, EM);
      "CODE" 34152;
      "PROCEDURE" BAKSYMTRI1(A, N, N1, N2, VEC); "CODE" 34144;

      TFMSYMTRI1(A, N, D, B, BB, EM);
      VALSYMTRI(D, BB, N, 1, NUMVAL, VAL, EM);
      VECSYMTRI(D, B, N, 1, NUMVAL, VAL, VEC, EM);
      BAKSYMTRI1(A, N, 1, NUMVAL, VEC)
"END" EIGSYM1;
      "EOP"

"CODE" 34162;
"COMMENT" MCA 2322;
"INTEGER" "PROCEDURE" QRIVALSYM2(A, N, VAL, EM); "VALUE" N;
"INTEGER" N; "ARRAY" A, VAL, EM;
"BEGIN" "ARRAY" B, BB[1:N];

      "PROCEDURE" TFMSYMTRI2(A, N, D, B, BB, EM); "CODE" 34140;
      "INTEGER" "PROCEDURE" QRIVALSYMTRI(D, BB, N, EM);
      "CODE" 34160;

      TFMSYMTRI2(A, N, VAL, B, BB, EM);
      QRIVALSYM2:= QRIVALSYMTRI(VAL, BB, N, EM)
"END" QRIVALSYM2;
      "EOP"

```

```

"CODE" 34163;
"COMMENT" MCA 2323;
"INTEGER" "PROCEDURE" GRISYM(A, N, VAL, EM); "VALUE" N;
"INTEGER" N; "ARRAY" A, VAL, EM;
"BEGIN" "ARRAY" B, BB[1:N];

      "PROCEDURE" TFMSYMTRI2(A, N, D, B, BB, EM); "CODE" 34140;
      "PROCEDURE" TFMPREVEC(A, N); "CODE" 34142;
      "INTEGER" "PROCEDURE" GRISYMTRI(A, N, D, B, BB, EM);
      "CODE" 34161;

      TFMSYMTRI2(A, N, VAL, B, BB, EM); TFMPREVEC(A, N);
      GRISYM;= GRISYMTRI(A, N, VAL, B, BB, EM)
"END" GRISYM;
"EOP"

```

```

"CODE" 34164;
"COMMENT" MCA 2327;
"INTEGER" "PROCEDURE" QRIVALSYM1(A, N, VAL, EM); "VALUE" N;
"INTEGER" N; "ARRAY" A, VAL, EM;
"BEGIN" "ARRAY" B, BB[1 : N];

      "PROCEDURE" TFMSYMTRI1(A, N, D, B, BB, EM); "CODE" 34143;
      "INTEGER" "PROCEDURE" QRIVALSYMTRI(D, BB, N, EM);
      "CODE" 34160;

      TFMSYMTRI1(A, N, VAL, B, BB, EM);
      QRIVALSYM1;= QRIVALSYMTRI(VAL, BB, N, EM)
"END" QRIVALSYM1;
"EOP"

```

SECTION : 3.3.1.1.3.1

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BRIEF DESCRIPTION:

THIS SECTION CONTAINS THREE PROCEDURES FOR SORTING THE ELEMENTS OF A VECTOR AND CORRESPONDINGLY PERMUTING THE ELEMENTS OF A VECTOR OR A MATRIX ROW.

- A) MERGESORT DELIVERS A PERMUTATION OF INDICES CORRESPONDING TO SORTING THE ELEMENTS OF A GIVEN VECTOR INTO NON-DECREASING ORDER.
- B) VECPERM PERMUTES THE ELEMENTS OF A GIVEN VECTOR CORRESPONDING TO A GIVEN PERMUTATION OF INDICES.
- C) ROWPERM PERMUTES THE ELEMENTS OF A GIVEN ROW OF A MATRIX CORRESPONDING TO A GIVEN PERMUTATION OF INDICES.

KEYWORDS:  
SORTING,  
PERMUTING.

SUBSECTION: MERGESORT.

CALLING SEQUENCE:

THE DECLARATION OF THE PROCEDURE IN THE CALLING PROGRAM READS:

```
"PROCEDURE" MERGESORT(VEC1,VEC2,LOW,UPP);  
"VALUE" LOW,UPP;"INTEGER" LOW,UPP;"ARRAY" VEC1,VEC2;  
"CODE" 36405;
```

THE MEANING OF THE FORMAL PARAMETERS IS:

VEC1 : <ARRAY IDENTIFIER>;  
"ARRAY" VEC1[LOW;UPP];  
ENTRY: THE VECTOR TO BE SORTED INTO  
NONDECREASING ORDER;  
EXIT: THE CONTENTS OF VEC1 ARE LEFT INVARIANT;

VEC2 : <ARRAY IDENTIFIER>;  
"INTEGER" "ARRAY" VEC2[LOW;UPP];  
EXIT: THE PERMUTATION OF INDICES CORRESPONDING TO  
SORTING THE ELEMENTS OF VEC1 INTO  
NON-DECREASING ORDER;

LOW : <ARITHMETIC EXPRESSION>;  
THE LOWER INDEX OF THE ARRAYS VEC1 AND VEC2;

UPP : <ARITHMETIC EXPRESSION>;  
THE UPPER INDEX OF THE ARRAYS VEC1 AND VEC2;

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PROCEDURES USED: NONE.

REQUIRED CENTRAL MEMORY: ONE LOCAL INTEGER ARRAY OF  
LENGTH N, WHERE  $N = UPP - LOW + 1$ .

RUNNING TIME: AVERAGE PROPORTIONAL TO  $N * LN(N)$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SORTING BY MERGING. ([1], [2])

EXAMPLE OF USE: THE PROCEDURE MERGESORT IS USED IN SYMEIGIMP  
(SECTION 3.3.1.1.3.3).

SUBSECTION: VECPERM.

CALLING SEQUENCE:

THE DECLARATION OF THE PROCEDURE IN THE CALLING PROGRAM READS:

```
"PROCEDURE" VECPERM(PERM, LOW, UPP, VECTOR);  
"VALUE" LOW, UPP; "INTEGER" LOW, UPP;  
"INTEGER" "ARRAY" PERM; "ARRAY" VECTOR;  
"CODE" 36404;
```

THE MEANING OF THE FORMAL PARAMETERS IS:

```
PERM :<ARRAY IDENTIFIER>;  
      "INTEGER" "ARRAY" PERM[LOW:UPP];  
      ENTRY: A GIVEN PERMUTATION (E.G. AS PRODUCED BY  
LOW :<ARITHMETIC EXPRESSION>;  
      THE LOWER INDEX OF THE ARRAYS PERM AND VECTOR;  
UPP :<ARITHMETIC EXPRESSION>;  
      THE UPPER INDEX OF THE ARRAYS PERM AND VECTOR;  
VECTOR :<ARRAY IDENTIFIER>;  
        "ARRAY" VECTOR[LOW:UPP];  
        ENTRY: THE REAL VECTOR TO BE PERMUTED;  
        EXIT: THE PERMUTED VECTOR ELEMENTS.
```

PROCEDURE USED: NONE.

REQUIRED CENTRAL MEMORY :  
ONE LOCAL BOOLEAN ARRAY OF LENGTH N IS DECLARED.

RUNNING TIME: PROPORTIONAL TO N.

LANGUAGE: ALGOL 60.

EXAMPLE OF USE: THE PROCEDURE VECPERM IS USED IN SYMEIGIMP;  
(SECTION 3.3.1.1.3.3).

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SUBSECTION: ROWPERM.

CALLING SEQUENCE:

THE DECLARATION OF THE PROCEDURE IN THE CALLING PROGRAM READS:

```
"PROCEDURE" ROWPERM(PERM,LOW,UPP,I,MATRIX);  
"VALUE" LOW,UPP,I;"INTEGER" LOW,UPP,I;  
"INTEGER" "ARRAY" PERM;"ARRAY" MATRIX;  
"CODE" 36403;
```

THE MEANING OF THE FORMAL PARAMETERS IS:

```
PERM :<ARRAY IDENTIFIER>;  
      "INTEGER" "ARRAY" PERM[LOW:UPP];  
      ENTRY: A GIVEN PERMUTATION (E.G. AS PRODUCED BY  
      MERGESORT) OF THE NUMBERS IN THE ARRAY VECTOR;  
LOW :<ARITHMETIC EXPRESSION>;  
      THE LOWER INDEX OF THE ARRAY PERM;  
UPP :<ARITHMETIC EXPRESSION>;  
      THE UPPER INDEX OF THE ARRAY PERM;  
I :<ARITHMETIC EXPRESSION>;  
      THE ROW INDEX OF THE MATRIX ELEMENTS;  
MATRIX :<ARRAY IDENTIFIER>;  
        "ARRAY" MATRIX [I : I, LOW : UPP];  
        ENTRY: MATRIX [I, LOW : UPP] SHOULD CONTAIN THE  
        ELEMENTS TO BE PERMUTED;  
        EXIT: MATRIX [I, LOW : UPP] CONTAINS THE ROW OF  
        PERMUTED ELEMENTS;
```

PROCEDURES USED: NONE.

REQUIRED CENTRAL MEMORY:

ONE LOCAL BOOLEAN ARRAY OF LENGTH N IS DECLARED.

RUNNING TIME: PROPORTIONAL TO N, WHERE  $N = UPP - LOW + 1$ .

LANGUAGE: ALGOL 60.

EXAMPLE OF USE: THE PROCEDURE ROWPERM IS USED IN SYMEIGIMP.  
(SECTION 3.3.1.1.3.3).

REFERENCES:

- [1] D.E. KNUTH, THE ART OF COMPUTER PROGRAMMING,  
VOL. 3/ SORTING AND SEARCHING, ADDISON-WESLEY 1973.  
(SECTION 5.2.4 P.159-173).
- [2] A.V. AHO, J.E. HOPCROFT & J.D. ULLMAN,  
THE DESIGN AND ANALYSIS OF COMPUTER ALGORITHMS,  
ADDISON-WESLEY 1974.  
(SECTION I.N, P65-67).

## SOURCE TEXTS:

```

CODE" 36405;
"PROCEDURE" MERGESORT(A,P,LOW,UP); "VALUE" LOW,UP;
"INTEGER" LOW,UP; "ARRAY" A; "INTEGER" "ARRAY" P;
"BEGIN" "INTEGER" I,L,R,PL,PR,LO,STEP,STAP,UMLP1,UMSP1,REST,RESTV;
      "BOOLEAN" ROUT,LOUT; "INTEGER" "ARRAY" HP[LOW:UP];
      "PROCEDURE" MERGE(LO,LS,RS); "VALUE" LO,LS,RS; "INTEGER" LO,LS,RS;
      "BEGIN" L:=LO; R:=LO+LS; LOUT:=ROUT:= "FALSE";
            "FOR" I:=LO,I+1 "WHILE" "(LOUT "OR" ROUT) "DO"
            "BEGIN" PL:=P[I]; PR:=P[R]; "IF" A[PL]>A[PR] "THEN"
                  "BEGIN" HP[I]:=PR; R:=R+1; ROUT:=R=LO+LS+RS "END" "ELSE"
                  "BEGIN" HP[I]:=PL; L:=L+1; LOUT:=L=LO+LS "END"
            "END" FOR I;
            "IF" ROUT "THEN"
            "BEGIN" "FOR" I:=LO+LS-1 "STEP" -1 "UNTIL" L "DO"
                  P[I+RS]:=P[I]; R:=L+RS
            "END";
            "FOR" I:=R-1 "STEP" -1 "UNTIL" LO "DO" P[I]:=HP[I];
      "END" MERGE;
      "FOR" I:=LOW "STEP" 1 "UNTIL" UP "DO" P[I]:=I; RESTV:=0;
      UMLP1:=UP-LOW+1;
      "FOR" STEP:=1, STEP*2 "WHILE" STEP < UMLP1 "DO"
      "BEGIN" STAP:=2*STEP; UMSP1:=UP-STAP+1;
            "FOR" LO:=LOW "STEP" STAP "UNTIL" UMSP1 "DO"
            MERGE(LO,STEP,STEP); REST:=UP-LO+1;
            "IF" REST>RESTV & RESTV>0 "THEN" MERGE(LO,REST-RESTV,RESTV);
            RESTV:=REST
      "END" FOR STEP
"END" MERGESORT;

```



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```

"CODE" 36404;
"PROCEDURE" VECPERM(PERM,LOW,UPP,VECTOR);"VALUE" LOW,UPP;
"INTEGER" LOW,UPP;"INTEGER" "ARRAY" PERM;"REAL" "ARRAY" VECTOR;
"BEGIN" "INTEGER" T,J,K;"REAL" A;"BOOLEAN" "ARRAY" TODO[LOW:UPP];
  "FOR" T:=LOW "STEP" 1 "UNTIL" UPP "DO" TODO[T]:=TRUE;
  "FOR" T:=LOW "STEP" 1 "UNTIL" UPP "DO"
    "BEGIN" "IF" TODO[T] "THEN"
      "BEGIN" K:=T;A:=VECTOR[K];
        "FOR" J:=PERM[K] "WHILE" J#T "DO"
          "BEGIN" VECTOR[K]:=VECTOR[J];TODO[K]:=FALSE;K:=J
          "END";VECTOR[K]:=A;TODO[K]:=FALSE
        "END" CYCLE;
      "END" FOR T;
    "END" VECPERM;

```

```

"CODE" 36403;
"PROCEDURE" ROWPERM(PERM,LOW,UPP,I,MAT);"VALUE" LOW,UPP,I;
"INTEGER" LOW,UPP,I;"INTEGER" "ARRAY" PERM;"REAL" "ARRAY" MAT;
"BEGIN" "INTEGER" T,J,K;"REAL" A;"BOOLEAN" "ARRAY" TODO[LOW:UPP];
  "FOR" T:=LOW "STEP" 1 "UNTIL" UPP "DO" TODO[T]:=TRUE;
  "FOR" T:=LOW "STEP" 1 "UNTIL" UPP "DO"
    "BEGIN" "IF" TODO[T] "THEN"
      "BEGIN" K:=T;A:=MAT[I,K];
        "FOR" J:=PERM[K] "WHILE" J#T "DO"
          "BEGIN" MAT[I,K]:=MAT[I,J];TODO[K]:=FALSE;K:=J
          "END";MAT[I,K]:=A;TODO[K]:=FALSE
        "END" CYCLE;
      "END" FOR T;
    "END" ROWPERM;

```

SECTION : 3.3.1.1.3.2

(NOVEMBER 1976)

PAGE 1

AUTHOR/CONTRIBUTOR: J.J.G. ADMIRAAL.

INSTITUTE: UNIVERSITY OF AMSTERDAM.

RECEIVED: 761101.

BRIEF DESCRIPTION:

THE PROCEDURE ORTHOG ORTHOGONALIZES SOME ADJACENT MATRIX COLUMNS ACCORDING TO THE MODIFIED GRAM SCHMIDT METHOD (SEE [1]).

KEYWORDS:

MATRIX COLUMNS,  
MODIFIED GRAM SCHMIDT ORTHOGONALIZATION.

CALLING SEQUENCE:

THE DECLARATION OF THE PROCEDURE IN THE CALLING PROGRAM READS:

```
"PROCEDURE" ORTHOG(N,LC,UC,X);  
"VALUE" N,LC,UC; "INTEGER" N,LC,UC;"ARRAY" X;  
"CODE" 36402;
```

THE MEANING OF THE FORMAL PARAMETERS IS:

```
N      : <ARITHMETIC EXPRESSION>;  
        THE ORDER OF THE MATRIX X;  
LC     : <ARITHMETIC EXPRESSION>;  
        THE LOWER COLUMN INDEX OF THE MATRIX COLUMNS;  
UC     : <ARITHMETIC EXPRESSION>;  
        THE UPPER COLUMN INDEX OF THE MATRIX COLUMNS;  
X      : <ARRAY IDENTIFIER>;  
        "ARRAY" X[1:N,LC:UC];  
        ENTRY: THE MATRIX COLUMNS, TO BE  
               ORTHOGONALIZED;  
        EXIT: THE ORTHOGONALIZED MATRIX COLUMNS.
```

PROCEDURES USED:

```
TAMMAT = CP34014,  
ELMCOL = CP34023.
```

REQUIRED CENTRAL MEMORY: NO LOCAL ARRAYS ARE DECLARED.

RUNNING TIME: PROPORTIONAL TO  $N \times 3$ .

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LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE MODIFIED GRAM SCHMIDT METHOD (SEE [1], CHAPTER 4.54).

EXAMPLE OF USE: THE PROCEDURE ORTHOG IS USED IN SYMEIGIMP.  
(SECTION 3.3.1.1.3.3).

REFERENCES:

- [1] J. H. WILKINSON.  
THE ALGEBRAIC EIGENVALUE PROBLEM.  
CLARENDON PRESS, OXFORD, 1965.

SOURCE TEXT:

```

"CODE" 36402;
"PROCEDURE" ORTHOG(N,LC,UC,X); "VALUE" N,LC,UC;
"INTEGER" N,LC,UC; "ARRAY" X;
"BEGIN" "INTEGER" I,J,K; "REAL" NORMX;
  "REAL" "PROCEDURE" TAMMAT(L,U,I,J,A,B); "CODE" 34014;
  "PROCEDURE" ELMCOL(L,U,I,J,A,B,X); "CODE" 34023;
  "FOR" J:=LC "STEP" 1 "UNTIL" UC "DO"
  "BEGIN" NORMX:=SQRT(TAMMAT(1,N,J,J,X,X));
    "FOR" I:=1 "STEP" 1 "UNTIL" N "DO" X[I,J]:=X[I,J]/NORMX;
    "FOR" K:=J+1 "STEP" 1 "UNTIL" UC "DO"
      ELMCOL(1,N,K,J,X,X,-TAMMAT(1,N,K,J,X,X))
  "END"
"END" ORTHOG;

```

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PAGE 1

AUTHOR/CONTRIBUTOR: J.J.G. ADMIRAAL.

INSTITUTE: UNIVERSITY OF AMSTERDAM.

RECEIVED: 761101.

BRIEF DESCRIPTION:

THE PROCEDURE SYMEIGIMP IMPROVES A GIVEN APPROXIMATION OF A REAL SYMMETRIC EIGENSYSTEM AND CALCULATES ERROR BOUNDS FOR THE EIGENVALUES.

KEYWORDS:

EIGENVALUES.  
EIGENVECTORS.  
SYMMETRIC MATRIX.  
RAYLEIGH QUOTIENTS.  
ERROR BOUNDS.  
IMPROVED EIGENSYSTEM.

CALLING SEQUENCE:

THE DECLARATION OF THE PROCEDURE IN THE CALLING PROGRAM READS:

```
"PROCEDURE" SYMEIGIMP(N,A,VEC,VAL1,VAL2,LBOUND,UBOUND,AUX);  
"VALUE" N;"INTEGER" N;  
"ARRAY" A,VEC,VAL1,VAL2,LBOUND,UBOUND,AUX;  
"CODE" 36401;
```

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF MATRIX A;  
A: <ARRAY IDENTIFIER>;  
"ARRAY" A[1:N,1:N] CONTAINS A REAL SYMMETRIC MATRIX  
WHOSE EIGENSYSTEM HAS TO BE IMPROVED;  
VEC: <ARRAY IDENTIFIER>;  
"ARRAY" VEC[1:N,1:N] CONTAINS A MATRIX WHOSE COLUMNS ARE  
A SYSTEM OF APPROXIMATE EIGENVECTORS OF MATRIX A;  
ENTRY: INITIAL APPROXIMATIONS;  
EXIT: IMPROVED APPROXIMATIONS;  
VAL1: <ARRAY IDENTIFIER>;  
"ARRAY" VAL1[1:N];  
ENTRY: INITIAL APPROXIMATIONS OF THE EIGENVALUES OF A;  
EXIT: THE HEAD PARTS OF THE DOUBLE PRECISION IMPROVED  
APPROXIMATIONS OF THE EIGENVALUES OF A;  
VAL2: <ARRAY IDENTIFIER>;  
"ARRAY" VAL2[1:N];  
EXIT: THE TAIL PARTS OF THE DOUBLE PRECISION  
IMPROVED EIGENVALUES OF A;

LBOUND,  
 UBOUND: <ARRAY IDENTIFIER>;  
 EXIT: "ARRAY" LBOUND, UBOUND [1:N] CONTAIN THE LOWER  
 AND UPPER ERRORBOUNDS RESPECTIVELY FOR THE EIGENVALUE  
 APPROXIMATIONS IN VAL1, VAL2 [1:N] SUCH THAT THE  
 I-TH EXACT EIGENVALUE LIES BETWEEN VAL1 [I] + VAL2 [I]  
 - LBOUND [I] AND VAL1 [I] + VAL2 [I] + UBOUND [I];  
 AUX: <ARRAY IDENTIFIER>;  
 "ARRAY" AUX [0:5];  
 ENTRY: AUX [0]: THE RELATIVE PRECISION OF THE ELEMENTS OF A;  
 AUX [2]: THE RELATIVE TOLERANCE FOR THE RESIDUAL MATRIX;  
 THE ITERATION ENDS WHEN THE MAXIMUM ABSOLUTE  
 VALUE OF THE RESIDU ELEMENTS IS SMALLER THAN  
 AUX [2] \* AUX [1].  
 AUX [4]: THE MAXIMUM NUMBER OF ITERATIONS ALLOWED;  
 EXIT: AUX [1]: INFINITY NORM OF THE MATRIX A;  
 AUX [3]: MAXIMUM ABSOLUTE ELEMENT OF THE RESIDUAL MATRIX;  
 AUX [5]: NUMBER OF ITERATIONS;

## PROCEDURES USED:

LNGMATVEC = CP34411,  
 LNGMATMAT = CP34413,  
 LNGTAMMAT = CP34414,  
 VECVEC = CP34010,  
 MATMAT = CP34013,  
 TAMMAT = CP34014,  
 MERGESORT = CP36405,  
 VECPERM = CP36404,  
 ROWPERM = CP36403,  
 ORTHOG = CP36402.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

REQUIRED CENTRAL MEMORY: AUXILIARY ARRAYS ARE DECLARED TO A  
 TOTAL OF  $3 * N * N + 6 * N$  REALS AND N INTEGERS.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE [1].

## REFERENCES:

- [1]. J. J. G. ADMIRAAL.  
ITERATIEF VERBETEREN VAN REEEL SYMMETRISCH EIGENSTEEEM  
EN BEREKENEN VAN FOUTGRENZEN VOOR DE VERKREGEN EIGENWAARDEN.  
DOCTORAL SCRIPTIION, MARCH 1976,  
UNIVERSITEIT VAN AMSTERDAM.
- [2]. R. T. GREGORY AND D. L. KARNEY.  
A COLLECTION OF MATRICES FOR TESTING COMPUTATIONAL  
ALGORITHMS.

## EXAMPLE OF USE.

```

"BEGIN" "INTEGER" I, J; "REAL" S;
"ARRAY" A, X[1:4, 1:4], VAL1, VAL2, LBOUND, UBOUND[1:4], EM, AUX[0:5];
"PROCEDURE" SYMEIGIMP(N, A, X, VAL1, VAL2, LBOUND, UBOUND, AUX);
"CODE" 36401;
"INTEGER" "PROCEDURE" QRISYM(A, N, VAL, EM); "CODE" 34163;
A[1, 1] := A[2, 2] := A[3, 3] := A[4, 4] := 6;
A[1, 2] := A[2, 1] := A[3, 1] := A[1, 3] := 4;
A[4, 2] := A[2, 4] := A[3, 4] := A[4, 3] := 4;
A[1, 4] := A[4, 1] := A[3, 2] := A[2, 3] := 1;
"FOR" I := 1 "STEP" 1 "UNTIL" 4 "DO"
"FOR" J := I "STEP" 1 "UNTIL" 4 "DO" X[I, J] := X[J, I] := A[I, J];
OUTPUT(61, "("("A"), /, 4(4(+DB), /))", A);
EM[0] := -14; EM[4] := 100; EM[2] := -5;
QRISYM(X, 4, VAL1, EM);
AUX[0] := 0; AUX[4] := 10; AUX[2] := -14;
SYMEIGIMP(4, A, X, VAL1, VAL2, LBOUND, UBOUND, AUX);
OUTPUT(61, ("/, "("THE EXACT EIGENVALUES ARE: -1 , +5 , +5 , +15")",
//,
"("THE DIFFERENCES BETWEEN THE CALCULATED AND THE EXACT EIGENVALUES"
), //, 4(N, /))", (VAL1[1]+1)+VAL2[1], (VAL1[2]-5)+VAL2[2], (VAL1[3]-
5)+VAL2[3], (VAL1[4]-15)+VAL2[4]);
OUTPUT(61, ("/, "("LOWERBOUNDS UPPERBOUNDS")", //"));
"FOR" I := 1 "STEP" 1 "UNTIL" 4 "DO"
OUTPUT(61, "("2(+D, D"+DDSB), /)", LBOUND[I], UBOUND[I]);
OUTPUT(61, ("/, "("NUMBER OF ITERATIONS = ")", ZD//,
"("INFINITY NORM OF A = ")", ZD//,
"("MAXIMUM ABSOLUTE ELEMENT OF RESIDU = ")", D, D"+DD"));
AUX[5], AUX[1], AUX[3]
"END" EXAMPLE OF USE

```

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DELIVERS:

A

+6	+4	+4	+1
+4	+6	+1	+4
+4	+1	+6	+4
+1	+4	+4	+6

THE EXACT EIGENVALUES ARE: -1 , +5 , +5 , +15

THE DIFFERENCES BETWEEN THE CALCULATED AND THE EXACT EIGENVALUES

-6.3423147029256"	=022
+5.5934784498910"	=018
+4.0389678347316"	=028
-5.5947317864427"	=018

LOWERBOUNDS    UPPERBOUNDS

+1.2"=23	+1.2"=23
+7.5"=09	+7.5"=09
+1.0"=13	+1.0"=13
+5.6"=18	+5.6"=18

NUMBER OF ITERATIONS = 2

INFINITY NORM OF A = 15

MAXIMUM ABSOLUTE ELEMENT OF RESIDU = 2.8"=14

## SOURCE TEXT:

```

"CODE" 36401;
"PROCEDURE" SYMEIGIMP(N,A,VEC,VAL1,VAL2,LBOUND,UBOUND,AUX);
"VALUE" N;"INTEGER" N;"ARRAY" A,VEC,VAL1,VAL2,LBOUND,UBOUND,AUX;
"BEGIN"
  "PROCEDURE" ORTHOG(N,LC,UC,X);"CODE" 36402;
  "PROCEDURE" MERGESORT(VEC1,VEC2,LOW,UPP);"CODE" 36405;
  "PROCEDURE" VECPERM(PERM,LOW,UPP,VECTOR);"CODE" 36404;
  "PROCEDURE" ROWPERM(PERM,LOW,UPP,MATRIX);"CODE" 36403;
  "INTEGER" K,I,J,I0,I1,ITER,MAXITP1;"REAL" S,HEAD,TAIL,MAX,TOL,
  MATEPS,RELEPRA,RELTOLR,NORMA;"INTEGER" "ARRAY" PERM[1:N];
  "ARRAY" P,P,Y[1:N,1:N],R0,R0T,EPS,Z,VAL3,ETA[1:N];
  "PROCEDURE" BOUNDS(I0,I1,N,LBOUND,UBOUND);"VALUE" I0,I1,N;
  "INTEGER" I0,I1,N;"ARRAY" LBOUND,UBOUND;
  "BEGIN" "INTEGER" K,I,J,I01;"REAL" EPS2,DL,DR;
    "FOR" I:=I0,I01 "WHILE" I<=I1 "DO"
      "BEGIN" J:=I01:=I;
        "FOR" J:=J+1 "WHILE" "IF" J>I1 "THEN" "FALSE" "ELSE"
          RQ[J]=RQ[J-1]+EPS[J]+EPS[J-1] "DO" I01:=J;
        "IF" I = I01 "THEN"
          "BEGIN"
            "IF" I<N "THEN"
              "BEGIN"
                "IF" I=1 "THEN" DL:=DR:=RQ[I+1]-RQ[I]-EPS[I+1]
                "ELSE" "BEGIN" DL:=RQ[I]-RQ[I-1]-EPS[I-1];
                DR:=RQ[I+1]-RQ[I]-EPS[I+1]
                "END"
              "END" "ELSE" DL:=DR:=RQ[I]-RQ[I-1]-EPS[I-1];
              EPS2:=EPS[I]*EPS[I];LBOUND[I]:=EPS2/DR+MATEPS;
              UBOUND[I]:=EPS2/DL+MATEPS
            "END" "ELSE"
              "BEGIN" "FOR" K:=I "STEP" 1 "UNTIL" I01 "DO"
                LBOUND[K]:=UBOUND[K]:=EPS[K]+MATEPS
              "END";I01:=I01+1
            "END"
          "END" BOUNDS;
  "PROCEDURE" LNORMATVEC(L,U,I,A,B,C,CC,D,DD);"CODE" 34411;
  "PROCEDURE" LNORMATMAT(L,U,I,J,A,B,C,CC,D,DD);"CODE" 34414;
  "PROCEDURE" LNORMATMAT(L,U,I,J,A,B,C,CC,D,DD);"CODE" 34413;
  "INTEGER" "PROCEDURE" ORISY(A,N,VAL,EM);"CODE" 34163;
  "REAL" "PROCEDURE" VECVEC(L,N,SHIFT,A,B);"CODE" 34010;
  "REAL" "PROCEDURE" MATMAT(L,N,I,J,A,B);"CODE" 34013;
  "REAL" "PROCEDURE" TANMAT(L,N,I,J,A,B);"CODE" 34014;
  "REAL" "PROCEDURE" INFRMAT(LC,UC,LP,UR,K,A);"CODE" 31064;
  "BOOLEAN" STOP;STOP:="FALSE";NORMA:=INFRMAT(1,N,1,N,S,A);
  RELEPRA:=AUX[0];RELTOLR:=AUX[2];MAXITP1:=AUX[3]+1;
  MATEPS:=RELEPRA*NORMA;TOL:=RELTOLR+NORMA;
  "FOR" ITER:=1 "STEP" 1 "UNTIL" MAXITP1 "DO"
  "BEGIN" STOP:="TRUE";MAX:=0;

```

"COMMENT"



```

"FOR" J:=1 "STEP" 1 "UNTIL" N "DO"
"FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
"BEGIN"
  LNGMATVEC(J, J, I, VEC, VAL1, 0, 0, HEAD, TAIL);
  LNGMATMAT(1, N, I, J, A, VEC, =HEAD, =TAIL, R[I, J], TAIL);
  "IF" ABS(R[I, J]) > MAX "THEN" MAX:=ABS(R[I, J])
"END"; "IF" MAX > TOL "THEN" STOP:=FALSE;
"IF" "NOT" STOP "AND" ITER < MAXITP1 "THEN"
"BEGIN"
  "FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
  LNGTAMMAT(1, N, I, I, VEC, R, VAL1[I], 0, RQ[I], RQT[I]);
  "FOR" J:=1 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" "FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
    ETA[I]:=R[I, J]-(RQ[J]-VAL1[J])*VEC[I, J];
    Z[J]:=SQRT(VECVEC(1, N, 0, ETA, ETA))
  "END";
  MERGESORT(RQ, PERM, 1, N); VECPERM(PERM, 1, N, RQ);
  "FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" EPS[I]:=Z[PERM[I]]; VAL3[I]:=VAL1[PERM[I]];
    ROWPERM(PERM, 1, N, I, VEC); ROWPERM(PERM, 1, N, I, R)
  "END";
  "FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
  "FOR" J:=I "STEP" 1 "UNTIL" N "DO"
  P[I, J]:=P[J, I]:=TAMMAT(1, N, I, J, VEC, R);
"END";
"FOR" IO:=1, I1+1 "WHILE" IO <= N "DO"
"BEGIN" J:=I1:=IO;
  "FOR" J:=J+1 "WHILE" "IF" J > N "THEN" "FALSE" "ELSE"
  RQ[J]-RQ[J-1] <= SORT((EPS[J]+EPS[J-1])*NORMA) "DO" I1:=J;
  "IF" STOP "OR" ITER=MAXITP1 "THEN"
  SOUNDS(IO, I1, N, LBOUND, UBOUND) "ELSE"
  "BEGIN"
    "IF" IO=I1 "THEN"
    "BEGIN" "FOR" K:=1 "STEP" 1 "UNTIL" N "DO"
      "IF" K=IO "THEN" Y[K, IO]:=1 "ELSE"
      R[K, IO]:=P[K, IO];
      VAL1[IO]:=RQ[IO]; VAL2[IO]:=RQT[PERM[IO]]
    "END" "ELSE"
    "BEGIN" "INTEGER" N1, IOM1, I1P1; "REAL" M1; "ARRAY" EM[0:5];
      N1:=I1-IO+1; EM[0]:=EM[2]:=-14; EM[4]:=10*N1;
      "BEGIN" "ARRAY" PP[1:N1, 1:N1], VAL4[1:N1]; M1:=0;
        "FOR" K:=IO "STEP" 1 "UNTIL" I1 "DO"
          M1:=M1+VAL3[K]; N1:=M1/N1;
    "END"
  "END"
"COMMENT"

```

```

"FOR" I:=1 "STEP" 1 "UNTIL" N1 "DO"
"FOR" J:=1 "STEP" 1 "UNTIL" N1 "DO"
"BEGIN" PP[I,J]:=P[I+IO-1,J+IO-1];
      "IF" I#J "THEN"
      PP[I,J]:=PP[I,J]+VAL3[J+IO-1]-M1
"END";"FOR" I:=IO "STEP" 1 "UNTIL" I1 "DO"
"BEGIN" VAL3[I]:=1;VAL1[I]:=RQ[I];
      VAL2[I]:=ROT[PERM[I]]
"END";
QRISYH(PP,N1,VAL4,EM);
MERGESORT(VAL4,PERM,1,N1);
"FOR" I:=1 "STEP" 1 "UNTIL" N1 "DO"
"FOR" J:=1 "STEP" 1 "UNTIL" N1 "DO"
P[I+IO-1,J+IO-1]:=PP[I,PERM[J]];
IOM1:=IO-1;I1P1:=I1+1;
"FOR" J:=IO "STEP" 1 "UNTIL" I1 "DO"
"BEGIN" "FOR" I:=1 "STEP" 1 "UNTIL" IOM1,
      I1P1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" S:=0;
      "FOR" K:=IO "STEP" 1 "UNTIL" I1 "DO"
      S:=S+P[I,K]*P[K,J];
      R[I,J]:=S
"END";"FOR" I:=IO "STEP" 1 "UNTIL" I1 "DO"
Y[I,J]:=P[I,J]
"END" FOR J
"END" INNERBLOCK
"END" I1>IO
"END" NOT STOP
"END" FOR IO;
"IF" "NOT" STOP "AND" ITER<MAXITP1 "THEN"
"BEGIN"
"FOR" J:=1 "STEP" 1 "UNTIL" N "DO"
"FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
"IF" VAL3[I]*=VAL3[J] "THEN"
Y[I,J]:=R[I,J]/(VAL3[J]-VAL3[I]);
"FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" "FOR" J:=1 "STEP" 1 "UNTIL" N "DO"
      Z[J]:=MATMAT(1,N,I,J,VEC,Y);
      "FOR" J:=1 "STEP" 1 "UNTIL" N "DO" VEC[I,J]:=Z[J]
"END";ORTHOG(N,1,N,VEC)
"END" "ELSE"
"BEGIN" AUX[5]:=ITER-1;"GOTO" EXIT "END"
"END" FOR ITER;
EXIT; AUX[1]:=NORNA;AUX[3]:=MAX
"END" SYMEIGMP;

```

SECTION 3.3.1.2.1

(JULY 1974)

PAGE 1

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BRIEF DESCRIPTION:

THIS SECTION CONTAINS FIVE PROCEDURES:

A) REAVALQRI CALCULATES THE EIGENVALUES OF A REAL UPPER-HESSENBERG MATRIX, PROVIDED THAT ALL EIGENVALUES ARE REAL, BY MEANS OF SINGLE QR ITERATION;

B) REAVECHES CALCULATES THE EIGENVECTOR CORRESPONDING TO A GIVEN REAL EIGENVALUE OF A REAL UPPER-HESSENBERG MATRIX BY MEANS OF INVERSE ITERATION;

C) REAQRI CALCULATES THE EIGENVALUES AND EIGENVECTORS OF A REAL UPPER-HESSENBERG MATRIX, PROVIDED THAT ALL EIGENVALUES ARE REAL, BY MEANS OF SINGLE QR ITERATION;

D) COMVALQRI CALCULATES THE REAL AND COMPLEX EIGENVALUES OF A REAL UPPER-HESSENBERG MATRIX BY MEANS OF DOUBLE QR ITERATION;

E) COMVECHES CALCULATES THE EIGENVECTOR CORRESPONDING TO A GIVEN COMPLEX EIGENVALUE OF A REAL UPPER-HESSENBERG MATRIX BY MEANS OF INVERSE ITERATION.

KEYWORDS:

EIGENVALUE,  
 EIGENVECTOR,  
 UPPER-HESSENBERG MATRIX,  
 QR ITERATION,  
 INVERSE ITERATION.

SUBSECTION: REAVALQRI.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "INTEGER" "PROCEDURE" REAVALQRI(A, N, EM, VAL); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, EM, VAL;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE ELEMENTS OF THE REAL UPPER-HESSSENBERG MATRIX  
 MUST BE GIVEN IN THE UPPER TRIANGLE AND THE FIRST  
 SUBDIAGONAL OF ARRAY A;  
 EXIT: THE HESSENBERG PART OF ARRAY A IS ALTERED;

N:  
 <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM:  
 <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EM[1], A NORM OF THE GIVEN MATRIX;  
 EM[2], THE RELATIVE TOLERANCE USED FOR THE QR  
 ITERATION;  
 IF THE ABSOLUTE VALUE OF SOME SUBDIAGONAL  
 ELEMENT IS SMALLER THAN EM[1] \* EM[2], THEN  
 THIS ELEMENT IS NEGLECTED AND THE MATRIX IS  
 PARTITIONED;  
 EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE  
 DATA TO BE GIVEN IN EM ARE:  
 EM[0] = "14,  
 EM[2] > EM[0] (E.G. EM[2] = "13),  
 EM[4] = 10 \* N;  
 EXIT: EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
 ELEMENTS NEGLECTED;  
 EM[5], THE NUMBER OF QR ITERATIONS PERFORMED;  
 IF THE ITERATION PROCESS IS NOT COMPLETED  
 WITHIN EM[4] ITERATIONS, THE VALUE EM[4] + 1  
 IS DELIVERED AND IN THIS CASE ONLY THE LAST  
 N - K ELEMENTS OF VAL ARE APPROXIMATE EIGEN-  
 VALUES OF THE GIVEN MATRIX, WHERE K IS  
 DELIVERED IN REAVALQRI;

VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:N];  
 THE EIGENVALUES OF THE GIVEN MATRIX ARE DELIVERED IN VAL.

MOREOVER:

REAVALQRI DELIVERS 0, PROVIDED THAT THE PROCESS IS COMPLETED WITHIN  
 EM[4] ITERATIONS; OTHERWISE REAVALQRI DELIVERS THE NUMBER OF EIGEN-  
 VALUES NOT CALCULATED.

## PROCEDURES USED:

ROTCOL = CP34040,  
ROTROW = CP34041.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

## METHOD AND PERFORMANCE:

THE METHOD USED IN THE PROCEDURE REAVALQRI IS THE SINGLE QR ITERATION OF FRANCIS (SEE REF[1], P. 54, REF[2] P. 515 - 543 AND REF[3]), THE EIGENVALUES OF A REAL UPPER-HESSSENBERG MATRIX ARE CALCULATED, PROVIDED THAT THE MATRIX HAS REAL EIGENVALUES ONLY.

## REFERENCES:

- [1], T.J. DEKKER AND W. HOFFMANN,  
ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2,  
MC TRACT 23, 1968, MATH. CENTR., AMSTERDAM.
- [2], J.H. WILKINSON,  
THE ALGEBRAIC EIGENVALUE PROBLEM,  
CLARENDON PRESS, OXFORD, 1965.
- [3], J.G. FRANCIS,  
THE QR TRANSFORMATION, PARTS 1 AND 2,  
COMP. J. 4 (1961), 265 - 271 AND 332 - 345.

## EXAMPLE OF USE:

THE PROCEDURE REAVALQRI IS USED IN REAEIGVAL, SECTION 3.3.1.2.2.

SUBSECTION: REAVECHES.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" REAVECHES(A, N, LAMBDA, EM, V); "VALUE" N, LAMBDA;  
 "INTEGER" N; "REAL" LAMBDA; "ARRAY" A, EM, V;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE ELEMENTS OF THE REAL UPPER-HESSSENBERG MATRIX  
 MUST BE GIVEN IN THE UPPER TRIANGLE AND THE FIRST  
 SUBDIAGONAL OF ARRAY A;  
 EXIT: THE HESSENBERG PART OF ARRAY A IS ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

LAMBDA: <ARITHMETIC EXPRESSION>;  
 THE GIVEN REAL EIGENVALUE OF THE UPPER-HESSSENBERG MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:9];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EM[1], A NORM OF THE GIVEN MATRIX;  
 EM[6], THE TOLERANCE USED FOR THE EIGENVECTOR; THE  
 INVERSE ITERATION ENDS IF THE EUCLIDIAN  
 NORM OF THE RESIDUE VECTOR IS SMALLER THAN  
 EM[1] \* EM[6];  
 EM[8], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE  
 DATA TO BE GIVEN IN EM ARE:  
 EM[0] = "-14,  
 EM[6] = "-10,  
 EM[8] = 5;

EXIT: EM[7], THE EUCLIDIAN NORM OF THE RESIDUE VECTOR OF  
 THE CALCULATED EIGENVECTOR;  
 EM[9], THE NUMBER OF INVERSE ITERATIONS PERFORMED;  
 IF EM[7] REMAINS LARGER THAN EM[1] \* EM[6]  
 DURING EM[8] ITERATIONS, THE VALUE EM[8] + 1  
 IS DELIVERED;

V: <ARRAY IDENTIFIER>;  
 "ARRAY" V[1:N];  
 THE CALCULATED EIGENVECTOR IS DELIVERED IN V,

PROCEDURES USED:

VECVEC = CP34010,  
 MATVEC = CP34011.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N SQUARED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE REAVECHES CALCULATES AN EIGENVECTOR CORRESPONDING TO A GIVEN APPROXIMATE REAL EIGENVALUE OF A REAL UPPER-HERSSENBERG MATRIX, BY MEANS OF INVERSE ITERATION (SEE REF [1], P. 55, REF [2], P. 619 - 629 AND REF [3]).

REFERENCES:

- [1], T. J. DEKKER AND W. HOFFMANN,  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2,  
 MC TRACT 23, 1968, MATH. CENTR., AMSTERDAM.
- [2], J. H. WILKINSON,  
 THE ALGEBRAIC EIGENVALUE PROBLEM,  
 CLARENDON PRESS, OXFORD, 1965.
- [3], J. M. VARAH,  
 EIGENVECTORS OF A REAL MATRIX BY INVERSE ITERATION,  
 STANFORD UNIVERSITY, TECH. REP. NO. CS 34, 1966.

EXAMPLE OF USE:

THE PROCEDURE REAVECHES IS USED IN REAEIG1, SECTION 3.3.1.2.2.

SUBSECTION: REAQR1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "INTEGER" "PROCEDURE" REAQR1(A, N, EM, VAL, VEC); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, EM, VAL, VEC;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE ELEMENTS OF THE REAL UPPER-HESSENBERG MATRIX  
 MUST BE GIVEN IN THE UPPER TRIANGLE AND THE FIRST  
 SUBDIAGONAL OF ARRAY A;  
 EXIT: THE HESSENBERG PART OF ARRAY A IS ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EM[1], A NORM OF THE GIVEN MATRIX;  
 EM[2], THE RELATIVE TOLERANCE USED FOR THE QR  
 ITERATION;  
 IF THE ABSOLUTE VALUE OF SOME SUBDIAGONAL  
 ELEMENT IS SMALLER THAN EM[1] \* EM[2], THEN  
 THIS ELEMENT IS NEGLECTED AND THE MATRIX IS  
 PARTITIONED;  
 EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE  
 DATA TO BE GIVEN IN EM ARE:  
 EM[0] = "14,  
 EM[2] > EM[0] (E.G. EM[2] = "13),  
 EM[4] = 10 \* N;  
 EXIT: EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
 ELEMENTS NEGLECTED;  
 EM[5], THE NUMBER OF QR ITERATIONS PERFORMED;  
 IF THE ITERATION PROCESS IS NOT COMPLETED  
 WITHIN EM[4] ITERATIONS, THE VALUE EM[4] + 1  
 IS DELIVERED; IN THIS CASE ONLY THE LAST  
 N = K ELEMENTS OF VAL AND THE LAST N = K  
 COLUMNS OF VEC ARE APPROXIMATED EIGENVALUES  
 AND EIGENVECTORS OF THE GIVEN MATRIX, WHERE K  
 IS DELIVERED IN REAQR1;

VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:N];  
 THE EIGENVALUES OF THE GIVEN MATRIX ARE DELIVERED IN VAL;

VEC: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC[1:N,1:N];  
 THE CALCULATED EIGENVECTORS, CORRESPONDING TO THE EIGEN-  
 VALUES IN ARRAY VAL[1:N], ARE DELIVERED IN THE COLUMNS OF  
 ARRAY VEC.



MOREOVER:

REAGRI DELIVERS 0, PROVIDED THAT THE PROCESS IS COMPLETED WITHIN EM(4) ITERATIONS; OTHERWISE REAGRI DELIVERS THE NUMBER OF EIGENVALUES AND EIGENVECTORS NOT CALCULATED.

PROCEDURES USED:

MATVEC = CP34011,  
 ROTCOL = CP34040,  
 ROTROW = CP34041.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE REAGRI CALCULATES THE EIGENVALUES OF AN UPPER-HESSENBERG MATRIX BY MEANS OF SINGLE QR ITERATION (SEE METHOD AND PERFORMANCE OF REAVALGRI, THIS SECTION). THE EIGENVECTORS ARE CALCULATED BY A DIRECT METHOD (SEE REF [1], P. 55-56), IN CONTRAST WITH REAVECHES WHICH USES INVERSE ITERATION. IF THE HESSENBERG MATRIX IS NOT TOO ILL-CONDITIONED WITH RESPECT TO ITS EIGENVALUE PROBLEM, THEN THIS METHOD YIELDS NUMERICALLY INDEPENDENT EIGENVECTORS AND IS COMPETITIVE WITH INVERSE ITERATION AS TO ACCURACY AND COMPUTATION TIME. IF THE QR ITERATION PROCESS IS NOT COMPLETED WITHIN THE GIVEN NUMBER OF ITERATIONS, NOT ALL EIGENVALUES AND EIGENVECTORS ARE DELIVERED. THE PROCEDURE REAGRI SHOULD BE USED ONLY IF ALL EIGENVALUES ARE REAL.

REFERENCES:

- [1]. T.J. DEKKER AND W. HOFFMANN,  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2,  
 MC TRACT 23, 1968, MATH. CENTR., AMSTERDAM.

EXAMPLE OF USE:

THE PROCEDURE REAGRI IS USED IN REAEIG3, SECTION 3.3.1.2.2.

## SUBSECTION: COMVALQRI.

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "INTEGER" "PROCEDURE" COMVALQRI(A, N, EM, RE, IM); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, EM, RE, IM;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE ELEMENTS OF THE REAL UPPER-HESSSENBERG MATRIX  
 MUST BE GIVEN IN THE UPPER TRIANGLE AND THE FIRST  
 SUBDIAGONAL OF ARRAY A;  
 EXIT: THE HESSENBERG PART OF ARRAY A IS ALTERED;

N:  
 <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM:  
 <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EM[1], A NORM OF THE GIVEN MATRIX;  
 EM[2], THE RELATIVE TOLERANCE USED FOR THE QR  
 ITERATION;  
 IF THE ABSOLUTE VALUE OF SOME SUBDIAGONAL  
 ELEMENT IS SMALLER THAN EM[1] \* EM[2], THEN  
 THIS ELEMENT IS NEGLECTED AND THE MATRIX IS  
 PARTITIONED;  
 EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE  
 DATA TO BE GIVEN IN EM ARE:  
 EM[0] = "14,  
 EM[2] > EM[0] (E.G. EM[2] = "13),  
 EM[4] = 10 \* N;  
 EXIT: EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
 ELEMENTS NEGLECTED;  
 EM[5], THE NUMBER OF QR ITERATIONS PERFORMED;  
 IF THE ITERATION PROCESS IS NOT COMPLETED  
 WITHIN EM[4] ITERATIONS, THE VALUE EM[4] + 1  
 IS DELIVERED AND IN THIS CASE ONLY THE LAST  
 N \* K ELEMENTS OF RE AND IM ARE APPROXIMATE  
 EIGENVALUES OF THE GIVEN MATRIX, WHERE K IS  
 DELIVERED IN COMVALQRI;

RE, IM: <ARRAY IDENTIFIER>;  
 "ARRAY" RE, IM[1:N];  
 THE REAL AND IMAGINARY PARTS OF THE CALCULATED EIGENVALUES  
 OF THE GIVEN MATRIX ARE DELIVERED IN ARRAY RE, IM[1:N], THE  
 MEMBERS OF EACH NONREAL COMPLEX CONJUGATE PAIR BEING  
 CONSECUTIVE,

MOREOVER:

COMVALQRI DELIVERS 0, PROVIDED THAT THE PROCESS IS COMPLETED WITHIN  
 EM[4] ITERATIONS; OTHERWISE COMVALQRI DELIVERS THE NUMBER OF EIGEN-  
 VALUES NOT CALCULATED.

PROCEDURES USED: NONE.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE METHOD USED IN THE PROCEDURE COMVALQRI FOR CALCULATING THE REAL AND COMPLEX EIGENVALUES OF A REAL UPPER-HESSSENBERG MATRIX IS THE DOUBLE QR ITERATION OF FRANCIS (SEE REF[1], P. 74, REF[2] P. 528 - 537 AND REF[3]).

REFERENCES:

- [1]. T.J. DEKKER AND W. HOFFMANN.  
ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2.  
MC TRACT 23, 1968, MATH. CENTR., AMSTERDAM.
- [2]. J.H. WILKINSON.  
THE ALGEBRAIC EIGENVALUE PROBLEM.  
CLARENDON PRESS, OXFORD, 1965.
- [3]. J.G. FRANCIS.  
THE QR TRANSFORMATION, PARTS 1 AND 2.  
COMP. J. 4 (1961), 265 - 271 AND 332 - 345.

EXAMPLE OF USE:

THE COMPLEX EIGENVALUES AND  $\alpha$ -VECTORS OF H, WITH  $N = 4$  AND  $H[I, J] =$   
"IF"  $I = 1$  "THEN"  $\alpha$  "ELSE" "IF"  $I = J = 1$  "THEN" 1 "ELSE" 0, MAY  
BE OBTAINED BY THE FOLLOWING PROGRAM:

```
"BEGIN" "INTEGER" I, J, M;
  "ARRAY" A[1:4, 1:4], RE, IM[1:4], EM[0:9];
  "INTEGER" "PROCEDURE" COMVALQRI(A, N, EM, RE, IM);
  "CODE" 34190;
  "PROCEDURE" COMVECHES(A, N, LAMBDA, MU, EM, U, V);
  "CODE" 34191;

  EM[0] := "-14; EM[2] := "-13; EM[1] := 4; EM[4] := 40;
  EM[6] := "-10; EM[8] := 5;
  "FOR" I := 1, 2, 3, 4 "DO" "FOR" J := 1, 2, 3, 4 "DO" A[I, J] :=
  "IF"  $I = 1$  "THEN"  $\alpha$  "ELSE" "IF"  $I = J = 1$  "THEN" 1 "ELSE" 0;
  M := COMVALQRI(A, 4, EM, RE, IM); OUTPUT(61, "("D, /")", M);
```

```

"FOR" J:= M + 1 "STEP" 1 "UNTIL" 4 "DO"
"BEGIN" "INTEGER" K; "ARRAY" U, V[1:4];
  "FOR" I:= 1, 2, 3, 4 "DO" "FOR" K:= 1, 2, 3, 4 "DO"
    A[I,K]:= "IF" I = 1 "THEN" 1 "ELSE"
    "IF" I = K = 1 "THEN" 1 "ELSE" 0;
    COMVECHES(A, 4, RE[J], IM[J], EM, U, V);
    OUTPUT(61, "( "/, 2(+,13D"+2D, 2B), 2/" )", RE[J], IM[J]);
    "FOR" I:= 1, 2, 3, 4 "DO"
      OUTPUT(61, "( "21B, 2(+,13D"+2D, 2B), /" )", U[I], V[I])
    "END";
  OUTPUT(61, "( "/, 2(,2D"+2D, /), 2(ZD, /)" )",
  EM[3], EM[7], EM[5], EM[9])
"END"

```

THE PROGRAM DELIVERS (THE RESULTS ARE CORRECT UP TO TWELVE DIGITS):

THE NUMBER OF NOT CALCULATED EIGENVALUES: 0

THE EIGENVALUES AND -VECTORS:

+ .3090169943750"+00	+ .9510565162952"+00		
		- .2527643931136"+00	+ .4314048696688"+00
		- .4883989055049"+00	+ .1070817869743"+00
		- .4908273055667"+01	+ .4975850535950"+00
		+ .4580641097602"+00	+ .2004426884413"+00
+ .3090169943750"+00	- .9510565162952"+00		
		- .2527643931136"+00	+ .4314048696688"+00
		- .4883989055049"+00	+ .1070817869743"+00
		- .4908273055667"+01	+ .4975850535950"+00
		+ .4580641097602"+00	+ .2004426884413"+00
- .8090169943749"+00	+ .5877852522924"+00		
		+ .1095191711534"+00	- .4878581260468"+00
		- .3753586823743"+00	+ .3303117611685"+00
		+ .4978239349006"+00	- .4659753040772"+01
		- .4301373647081"+00	+ .2549153731770"+00
- .8090169943749"+00	- .5877852522924"+00		
		+ .1095191711534"+00	+ .4878581260468"+00
		- .3753586823743"+00	+ .3303117611685"+00
		+ .4978239349006"+00	+ .4659753040772"+01
		- .4301373647081"+00	+ .2549153731770"+00

THE ARRAY EM: EM[3] = .67"=22  
 EM[7] = .17"=13  
 EM[5] = 9  
 EM[9] = 1 .

SUBSECTION: COMVECHES.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" COMVECHES(A, N, LAMBDA, MU, EM, U, V);  
 "VALUE" N, LAMBDA, MU;  
 "INTEGER" N; "REAL" LAMBDA, MU; "ARRAY" A, EM, U, V;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE ELEMENTS OF THE REAL UPPER-HESSSENBERG MATRIX  
 MUST BE GIVEN IN THE UPPER TRIANGLE AND THE FIRST  
 SUBDIAGONAL OF ARRAY A;  
 EXIT: THE HESSENBERG PART OF ARRAY A IS ALTERED;

N:  
 <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

LAMBDA, MU:  
 <ARITHMETIC EXPRESSION>;  
 THE REAL AND IMAGINARY PART OF THE GIVEN EIGENVALUE;

EM:  
 <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:9];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EM[1], A NORM OF THE GIVEN MATRIX;  
 EM[6], THE TOLERANCE USED FOR THE EIGENVECTOR; THE  
 INVERSE ITERATION ENDS IF THE EUCLIDIAN  
 NORM OF THE RESIDUE VECTOR IS SMALLER THAN  
 EM[1] \* EM[6];  
 EM[8], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE  
 DATA TO BE GIVEN IN EM ARE:  
 EM[0] = "14,  
 EM[6] = "10,  
 EM[8] = 5;  
 EXIT: EM[7], THE EUCLIDIAN NORM OF THE RESIDUE VECTOR OF  
 THE CALCULATED EIGENVECTOR;  
 EM[9], THE NUMBER OF INVERSE ITERATIONS PERFORMED;  
 IF EM[7] REMAINS LARGER THAN EM[1] \* EM[6]  
 DURING EM[8] ITERATIONS, THE VALUE EM[8] + 1  
 IS DELIVERED;

U, V: <ARRAY IDENTIFIER>;  
 "ARRAY" U, V[1:N];  
 THE REAL AND IMAGINARY PARTS OF THE CALCULATED EIGENVECTOR  
 ARE DELIVERED IN THE ARRAYS U, V[1:N].

SECTION 3,3,1,2,1

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PROCEDURES USED:

VECVEC = CP34010,  
 MATVEC = CP34011,  
 TAMVEC = CP34012.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N SQUARED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE PROCEDURE COMVECHES CALCULATES AN EIGENVECTOR CORRESPONDING TO A GIVEN APPROXIMATE EIGENVALUE OF A REAL UPPER-HESSENBERG MATRIX, BY MEANS OF INVERSE ITERATION (SEE REF[1], P. 75, REF[2], P. 629 - 633 AND REF[3]).

REFERENCES:

- [1]. T.J. DEKKER AND W. HOFFMANN,  
 ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2,  
 MC TRACT 23, 1968, MATH. CENTR., AMSTERDAM.
- [2]. J.H. WILKINSON,  
 THE ALGEBRAIC EIGENVALUE PROBLEM,  
 CLARENDON PRESS, OXFORD, 1965.
- [3]. J.M. VARAH,  
 EIGENVECTORS OF A REAL MATRIX BY INVERSE ITERATION,  
 STANFORD UNIVERSITY, TECH. REP. NO. CS 34, 1966.

EXAMPLE OF USE:

SEE EXAMPLE OF USE OF COMVALQRI, THIS SECTION.

SOURCE TEXT(S) :

```
"CODE" 34180;
"COMMENT" MCA 2410;
"INTEGER" "PROCEDURE" REAVALQRI(A, N, EM, VAL); "VALUE" N;
"INTEGER" N; "ARRAY" A, EM, VAL;
"BEGIN" "INTEGER" NI, I, I1, J, Q, MAX, COUNT;
"REAL" DET, W, SHIFT, KAPPA, NU, MU, R, TOL, DELTA, MACHTOL, S;

"PROCEDURE" ROTCOL(L, U, I, J, A, C, S); "CODE" 34040;
"PROCEDURE" ROTROW(L, U, I, J, A, C, S); "CODE" 34041;
"COMMENT"
```

```

MACHTOL:= EM[0] * EM[1]; TOL:= EM[1] * EM[2]; MAX:= EM[4];
COUNT:= 0; R:= 0;
IN: N1:= N - 1;
"FOR" I:= N, I - 1 "WHILE" ("IF" I >= 1 "THEN"
ABS(A[I + 1,I]) > TOL "ELSE" "FALSE") "DO" Q:= I;
"IF" Q > 1 "THEN"
"BEGIN" "IF" ABS(A[Q,Q - 1]) > R "THEN"
R:= ABS(A[Q,Q - 1])
"END";
"IF" Q = N "THEN"
"BEGIN" VAL[N]:= A[N,N]; N1:= N1 "END"
"ELSE"
"BEGIN" DELTA:= A[N,N] - A[N1,N1]; DET:= A[N,N] * A[N1,N];
"IF" ABS(DELTA) < MACHTOL "THEN" S:= SQRT(DET) "ELSE"
"BEGIN" W:= 2 / DELTA; S:= W * W * DET + 1;
S:= "IF" S <= 0 "THEN" -DELTA * .5 "ELSE"
W * DET / (SQRT(S) + 1)
"END";
"IF" Q = N1 "THEN"
"BEGIN" VAL[N]:= A[N,N] + S;
VAL[N1]:= A[N1,N1] - S; N1:= N - 2
"END"
"ELSE"
"BEGIN" COUNT:= COUNT + 1;
"IF" COUNT > MAX "THEN" "GOTO" OUT;
SHIFT:= A[N,N] + S; "IF" ABS(DELTA) < TOL "THEN"
"BEGIN" W:= A[N1,N1] - S;
"IF" ABS(W) < ABS(SHIFT) "THEN" SHIFT:= W
"END";
A[Q,Q]:= A[Q,Q] - SHIFT;
"FOR" I:= Q "STEP" 1 "UNTIL" N - 1 "DO"
"BEGIN" I1:= I + 1; A[I1,I1]:= A[I1,I1] - SHIFT;
KAPPA:= SQRT(A[I,I] ** 2 + A[I1,I1] ** 2);
"IF" I > Q "THEN"
"BEGIN" A[I,I - 1]:= KAPPA * NU;
W:= KAPPA * MU
"END"
"ELSE" W:= KAPPA; MU:= A[I,I] / KAPPA;
NU:= A[I1,I] / KAPPA; A[I,I]:= W;
ROTROW(I1, N, I, I1, A, MU, NU);
ROTCOL(Q, I, I, I1, A, MU, NU);
A[I,I]:= A[I,I] + SHIFT
"END";
A[N,N - 1]:= A[N,N] * NU; A[N,N]:= A[N,N] * MU + SHIFT
"END"
"END";
"IF" N > 0 "THEN" "GOTO" IN;
OUT: EM[3]:= R; EM[5]:= COUNT; REAVALQRI:= N
"END" REAVALQRI;
"EOP"

```

```

"CODE" 34181;
"COMMENT" MCA 2411;
"PROCEDURE" REAVECHES(A, N, LAMBDA, EM, V); "VALUE" N, LAMBDA;
"INTEGER" N; "REAL" LAMBDA; "ARRAY" A, EM, V;
"BEGIN" "INTEGER" I, I1, J, COUNT, MAX;
      "REAL" M, R, NORM, MACHTOL, TOL;
      "BOOLEAN" "ARRAY" P[1:N];

      "REAL" "PROCEDURE" VECVEC(L, U, SHIFT, A, B); "CODE" 34010;
      "REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;

      NORM:= EM[1]; MACHTOL:= EM[0] * NORM; TOL:= EM[6] * NORM;
      MAX:= EM[8]; A[1,1]:= A[1,1] + LAMBDA;
      GAUSS: "FOR" I:= 1 "STEP" 1 "UNTIL" N - 1 "DO"
        "BEGIN" I1:= I + 1; R:= A[I,I]; M:= A[I1,I];
          "IF" ABS(M) < MACHTOL "THEN" M:= MACHTOL;
          P[I]:= ABS(M) <= ABS(R);
          "IF" P[I] "THEN"
            "BEGIN" A[I1,I]:= M:= M / R;
              "FOR" J:= I1 "STEP" 1 "UNTIL" N "DO"
                A[I1,J]:= ("IF" J > I1 "THEN" A[I1,J]
                  "ELSE" A[I1,J] + LAMBDA) + M * A[I,J]
            "END"
          "ELSE"
            "BEGIN" A[I,I]:= M; A[I1,I]:= M:= R / M;
              "FOR" J:= I1 "STEP" 1 "UNTIL" N "DO"
                "BEGIN" R:= ("IF" J > I1 "THEN" A[I1,J] "ELSE"
                  A[I1,J] + LAMBDA);
                  A[I1,J]:= A[I,J] + M * R; A[I,J]:= R
                "END"
            "END"
        "END" GAUSS;
      "IF" ABS(A[N,N]) < MACHTOL "THEN" A[N,N]:= MACHTOL;
      "FOR" J:= 1 "STEP" 1 "UNTIL" N "DO" V[J]:= 1; COUNT:= 0;
      FORWARD: COUNT:= COUNT + 1; "IF" COUNT > MAX "THEN" "GOTO" OUT;
      "FOR" I:= 1 "STEP" 1 "UNTIL" N - 1 "DO"
        "BEGIN" I1:= I + 1;
          "IF" P[I] "THEN" V[I1]:= V[I1] + A[I1,I] * V[I] "ELSE"
            "BEGIN" R:= V[I1]; V[I1]:= V[I] + A[I1,I] * R;
              V[I]:= R
            "END"
        "END" FORWARD;
      BACKWARD: "FOR" I:= N "STEP" -1 "UNTIL" 1 "DO"
        V[I]:= (V[I] - MATVEC(I + 1, N, I, A, V)) / A[I,I];
        R:= 1 / SQRT(VECVEC(1, N, 0, V, V));
        "FOR" J:= 1 "STEP" 1 "UNTIL" N "DO" V[J]:= V[J] * R;
        "IF" R > TOL "THEN" "GOTO" FORWARD;
      OUT: EM[7]:= R; EM[9]:= COUNT
"END" REAVECHES;
"EOP"

```



```

"CODE" 34186;
"COMMENT" MCA 2416;
"INTEGER" "PROCEDURE" REAQR(A, N, EM, VAL, VEC); "VALUE" N;
"INTEGER" N; "ARRAY" A, EM, VAL, VEC;
"BEGIN" "INTEGER" M1, I, I1, M, J, Q, MAX, COUNT;
"REAL" W, SHIFT, KAPPA, NU, MU, R, TOL, S, MACHTOL,
ELMAX, T, DELTA, DET;
"ARRAY" TF[1:N];

"REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
"PROCEDURE" ROTCOL(L, U, I, J, A, C, S); "CODE" 34040;
"PROCEDURE" ROTROW(L, U, I, J, A, C, S); "CODE" 34041;

MACHTOL:= EM[0] * EM[1]; TOL:= EM[1] * EM[2]; MAX:= EM[4];
COUNT:= 0; ELMAX:= 0; M:= N;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" VEC[I,I]:= 1;
"FOR" J:= I + 1 "STEP" 1 "UNTIL" N "DO"
VEC[I,J]:= VEC[J,I]:= 0
"END";
IN: M1:= M - 1;
"FOR" I:= M, I - 1 "WHILE" ("IF" I >= 1 "THEN"
ABS(A[I + 1,I]) > TOL "ELSE" "FALSE") "DO" Q:= I;
"IF" Q > 1 "THEN"
"BEGIN" "IF" ABS(A[Q,Q - 1]) > ELMAX "THEN"
ELMAX:= ABS(A[Q, Q - 1])
"END";
"IF" Q = M "THEN"
"BEGIN" VAL[M]:= A[M,M]; M:= M1 "END"
"ELSE"
"BEGIN" DELTA:= A[M,M] - A[M1,M1]; DET:= A[M,M1] * A[M1,M];
"IF" ABS(DELTA) < MACHTOL "THEN" S:= SQRT(DET) "ELSE"
"BEGIN" W:= 2 / DELTA; S:= W * W * DET + 1;
S:= "IF" S <= 0 "THEN" -DELTA * .5 "ELSE"
W * DET / (SQRT(S) + 1)
"END";
"IF" Q = M1 "THEN"
"BEGIN" A[M,M]:= VAL[M]:= A[M,M] + S;
A[Q,Q]:= VAL[Q]:= A[Q,Q] - S;
T:= "IF" ABS(S) < MACHTOL "THEN"
(S + DELTA) / A[M,Q] "ELSE" A[Q,M] / S;
R:= SQRT(T * T + 1); NU:= 1 / R;
MU:= -T * NU; A[Q,M]:= A[Q,M] - A[M,Q];
ROTROW(Q + 2, N, Q, M, A, MU, NU);
ROTCOL(1, Q - 1, Q, M, A, MU, NU);
ROTCOL(1, N, Q, M, VEC, MU, NU); M:= M - 2
"END"
    
```

```

"ELSE"
"BEGIN" COUNT:= COUNT + 1;
"IF" COUNT > MAX "THEN" "GOTO" END;
SHIFT:= A[M,M] + S; "IF" ABS(DELTA) < TOL "THEN"
"BEGIN" W:= A[M1,M1] + S;
"IF" ABS(W) < ABS(SHIFT) "THEN" SHIFT:= W
"END";
A[Q,Q]:= A[Q,Q] + SHIFT;
"FOR" I:= Q "STEP" 1 "UNTIL" M1 "DO"
"BEGIN" I1:= I + 1; A[I1,I1]:= A[I1,I1] + SHIFT;
KAPPA:= SQRT(A[I,I] ** 2 + A[I1,I1] ** 2);
"IF" I > Q "THEN"
"BEGIN" A[I,I - 1]:= KAPPA * NU;
W:= KAPPA * MU
"END"
"ELSE" W:= KAPPA; MU:= A[I,I] / KAPPA;
NU:= A[I1,I] / KAPPA; A[I,I]:= W;
ROTRW(I1, N, I, I1, A, MU, NU);
ROTCOL(1, I, I, I1, A, MU, NU);
A[I,I]:= A[I,I] + SHIFT;
ROTCOL(1, N, I, I1, VEC, MU, NU)
"END";
A[M,M1]:= A[M,M] * NU; A[M,M]:= A[M,M] * MU + SHIFT
"END"
"END";
"IF" M > 0 "THEN" "GOTO" IN;
"FOR" J:= N "STEP" -1 "UNTIL" 2 "DO"
"BEGIN" TF[J]:= 1; T:= A[J,J];
"FOR" I:= J - 1 "STEP" -1 "UNTIL" 1 "DO"
"BEGIN" DELTA:= T - A[I,I];
TF[I]:= MATVEC(I + 1, J, I, A, TF) /
("IF" ABS(DELTA) < MACHTOL "THEN" MACHTOL "ELSE" DELTA)
"END";
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
VEC[I,J]:= MATVEC(1, J, I, VEC, TF)
"END";
END: EM[3]:= ELMAX; EM[5]:= COUNT; REAGRI:= M
"END" REAGRI;
"EOP"

```

```

"CODE" 34190;
"COMMENT" MCA 2420;
"INTEGER" "PROCEDURE" COMVALGRI(A, N, EM, RE, IM); "VALUE" N;
"INTEGER" N; "ARRAY" A, EM, RE, IM;
"BEGIN" "INTEGER" I, J, P, Q, MAX, COUNT, N1, P1, P2, IMIN1,
      I1, I2, I3;
      "REAL" DISC, SIGMA, RHO, G1, G2, G3, PSI1, PSI2, AA, E, K,
      S, NORM, MACHTOL2, TOL, W;
      "BOOLEAN" B;

      NORM:= EM[1]; MACHTOL2:= (EM[0] * NORM) ** 2;
      TOL:= EM[2] * NORM; MAX:= EM[4]; COUNT:= 0; W:= 0;
IN: "FOR" I:= N, I = 1 "WHILE"
      ("IF" I >= 1 "THEN" ABS(A[I + 1, I]) > TOL "ELSE" "FALSE")
      "DO" Q:= I; "IF" Q > 1 "THEN"
      "BEGIN" "IF" ABS(A[Q, Q - 1]) > W "THEN" W:= ABS(A[Q, Q - 1])
      "END";
      "IF" Q >= N - 1 "THEN"
      "BEGIN" N1:= N - 1; "IF" Q = N "THEN"
      "BEGIN" RE[N]:= A[N, N]; IM[N]:= 0; N:= N1 "END"
      "ELSE"
      "BEGIN" SIGMA:= A[N, N] * A[N1, N1];
      RHO:= -A[N, N1] * A[N1, N];
      DISC:= SIGMA ** 2 - 4 * RHO; "IF" DISC > 0 "THEN"
      "BEGIN" DISC:= SQRT(DISC);
      S:= -2 * RHO / (SIGMA + ("IF" SIGMA >= 0
      "THEN" DISC "ELSE" -DISC));
      RE[N]:= A[N, N] + S;
      RE[N1]:= A[N1, N1] - S; IM[N]:= IM[N1]:= 0
      "END"
      "ELSE"
      "BEGIN" RE[N]:= RE[N1]:= (A[N1, N1] + A[N, N]) / 2;
      IM[N1]:= SQRT(-DISC) / 2; IM[N]:= -IM[N1]
      "END";
      N:= N - 2
      "END"
"END"
"ELSE"
"BEGIN" COUNT:= COUNT + 1; "IF" COUNT > MAX "THEN"
      "GOTO" OUT; N1:= N - 1;
      SIGMA:= A[N, N] + A[N1, N1] + SQRT(ABS(A[N1, N - 2] * A[N, N1])
      * EM[0]); RHO:= A[N, N] * A[N1, N1] - A[N, N1] * A[N1, N];
      "FOR" I:= N - 1, I = 1 "WHILE"
      ("IF" I = 1 >= Q "THEN" ABS(A[I, I - 1]) *
      A[I1, I] * (ABS(A[I, I] + A[I1, I1]) - SIGMA) +
      ABS(A[I + 2, I1])) > ABS(A[I, I] * ((A[I, I] - SIGMA) +
      A[I, I1] * A[I1, I] + RHO)) * TOL
      "ELSE" "FALSE") "DO" P1:= I1:= I; P:= P1 - 1;
      P2:= P + 2;

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"COMMENT"

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"FOR" I:= P "STEP" 1 "UNTIL" N = 1 "DO"
"BEGIN" IMIN1:= I - 1; I1:= I + 1; I2:= I + 2;
"IF" I = P "THEN"
"BEGIN" G1:= A[P,P] * (A[P,P] = SIGMA) + A[P,P1] *
A[P1,P] + RHO;
G2:= A[P1,P] * (A[P,P] + A[P1,P1] = SIGMA);
"IF" P1 <= N1 "THEN"
"BEGIN" G3:= A[P1,P] * A[P2,P1]; A[P2,P]:= 0 "END"
"ELSE" G3:= 0
"END"
"ELSE"
"BEGIN" G1:= A[I,IMIN1]; G2:= A[I1,IMIN1];
G3:= "IF" I2 <= N "THEN" A[I2,IMIN1] "ELSE" 0
"END";
K:= "IF" G1 >= 0 "THEN"
SQRT(G1 ** 2 + G2 ** 2 + G3 ** 2) "ELSE"
-SQRT(G1 ** 2 + G2 ** 2 + G3 ** 2);
B:= ABS(K) > MACHTOL2;
AA:= "IF" B "THEN" G1 / K + 1 "ELSE" 2;
PSI1:= "IF" B "THEN" G2 / (G1 + K) "ELSE" 0;
PSI2:= "IF" B "THEN" G3 / (G1 + K) "ELSE" 0;
"IF" I = Q "THEN" A[I,IMIN1]:= "IF" I = P "THEN"
=A[I,IMIN1] "ELSE" =K;
"FOR" J:= I "STEP" 1 "UNTIL" N "DO"
"BEGIN" E:= AA * (A[I,J] + PSI1 * A[I1,J] +
("IF" I2 <= N "THEN" PSI2 * A[I2,J] "ELSE" 0));
A[I,J]:= A[I,J] + E; A[I1,J]:= A[I1,J] + PSI1 * E;
"IF" I2 <= N "THEN" A[I2,J]:= A[I2,J] + PSI2 * E
"END";
"FOR" J:= 0 "STEP" 1 "UNTIL"
("IF" I2 <= N "THEN" I2 "ELSE" N) "DO"
"BEGIN" E:= AA * (A[J,I] + PSI1 * A[J,I1] +
("IF" I2 <= N "THEN" PSI2 * A[J,I2] "ELSE" 0));
A[J,I]:= A[J,I] + E; A[J,I1]:= A[J,I1] + PSI1 * E;
"IF" I2 <= N "THEN" A[J,I2]:= A[J,I2] + PSI2 * E
"END";
"IF" I2 <= N1 "THEN"
"BEGIN" I3:= I + 3; E:= AA * PSI2 * A[I3,I2];
A[I3,I1]:= =E;
A[I3,I1]:= =PSI1 * E;
A[I3,I2]:= A[I3,I2] + PSI2 * E
"END"
"END"
"END"
"IF" N > 0 "THEN" "GOTO" IN;
OUT: EM[3]:= W; EM[5]:= COUNT; COMVALQRI:= N
"END" COMVALQRI;
"EQP"

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"CODE" 34191;
"COMMENT" MCA 2421;
"PROCEDURE" COMVECHES(A, N, LAMBDA, MU, EM, U, V);
"VALUE" N, LAMBDA, MU;
"INTEGER" N; "REAL" LAMBDA, MU; "ARRAY" A, EM, U, V;
"BEGIN" "INTEGER" I, I1, J, COUNT, MAX;
    "REAL" AA, BB, D, M, R, S, W, X, Y, NORM, MACHTOL, TOL;
    "ARRAY" G, F[1:N];
    "BOOLEAN" "ARRAY" P[1:N];

    "REAL" "PROCEDURE" VECVEC(L, U, SHIFT, A, B); "CODE" 34010;
    "REAL" "PROCEDURE" MATVEC(L, U, I, A, B); "CODE" 34011;
    "REAL" "PROCEDURE" TAMVEC(L, U, I, A, B); "CODE" 34012;

    NORM:= EM[1]; MACHTOL:= EM[0] * NORM; TOL:= EM[6] * NORM;
    MAX:= EM[8];
    "FOR" I:= 2 "STEP" 1 "UNTIL" N "DO"
    "BEGIN" F[I - 1]:= A[I, I - 1]; A[I, 1]:= 0 "END";
    AA:= A[1, 1] - LAMBDA; BB:= -MU;
    "FOR" I:= 1 "STEP" 1 "UNTIL" N - 1 "DO"
    "BEGIN" I1:= I + 1; M:= F[I];
        "IF" ABS(M) < MACHTOL "THEN" M:= MACHTOL;
        A[I, I1]:= M; D:= AA ** 2 + BB ** 2; P[I]:= ABS(M) < SQRT(D);
        "IF" P[I] "THEN"
        "BEGIN" "COMMENT" A[I, J] * FACTOR AND A[I1, J] = A[I, J];
            F[I]:= R:= M * AA / D; G[I]:= S:= -M * BB / D;
            W:= A[I1, I]; X:= A[I, I1]; A[I1, I1]:= Y:= X * S + W * R;
            A[I, I1]:= X:= X * R - W * S;
            AA:= A[I1, I1] - LAMBDA - X; BB:= -(MU + Y);
            "FOR" J:= I + 2 "STEP" 1 "UNTIL" N "DO"
            "BEGIN" W:= A[J, I]; X:= A[I, J];
                A[J, I1]:= Y:= X * S + W * R;
                A[I, J]:= X:= X * R - W * S; A[J, I1]:= -Y;
                A[I1, J]:= A[I1, J] - X
            "END"
        "END"
    "ELSE"
    "BEGIN" "COMMENT" INTERCHANGE A[I1, J] AND
        A[I, J] = A[I1, J] * FACTOR;
        F[I]:= R:= AA / M; G[I]:= S:= BB / M;
        W:= A[I1, I1] - LAMBDA; AA:= A[I, I1] - R * W - S * MU;
        A[I, I1]:= W; BB:= A[I1, I] - S * W + R * MU;
        A[I1, I]:= -MU;
        "FOR" J:= I + 2 "STEP" 1 "UNTIL" N "DO"
        "BEGIN" W:= A[I1, J]; A[I1, J]:= A[I, J] - R * W;
            A[I, J]:= W;
            A[J, I1]:= A[J, I] - S * W; A[J, I]:= 0
        "END"
    "END"
"END"

```

```

P[N]:= "TRUE"; D:= AA ** 2 + BB ** 2; "IF" D < MACHTOL ** 2
"THEN" "BEGIN" AA:= MACHTOL; BB:= 0; D:= MACHTOL ** 2 "END";
A[N,N]:= 0; F[N]:= AA; G[N]:= -BB;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" U[I]:= 1; V[I]:= 0 "END";
COUNT:= 0;
FORWARD: "IF" COUNT > MAX "THEN" "GOTO" OUTM;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" "IF" P[I] "THEN"
    "BEGIN" W:= V[I]; V[I]:= G[I] * U[I] + F[I] * W;
    U[I]:= F[I] * U[I] - G[I] * W; "IF" I < N "THEN"
    "BEGIN" V[I + 1]:= V[I + 1] - V[I];
    U[I + 1]:= U[I + 1] - U[I]
    "END"
"END"
"ELSE"
"BEGIN" AA:= U[I + 1]; BB:= V[I + 1];
    U[I + 1]:= U[I] - (F[I] * AA - G[I] * BB); U[I]:= AA;
    V[I + 1]:= V[I] - (G[I] * AA + F[I] * BB); V[I]:= BB
"END"
"END" FORWARD;
BACKWARD: "FOR" I:= N "STEP" -1 "UNTIL" 1 "DO"
"BEGIN" I1:= I + 1;
    U[I]:= (U[I] - MATVEC(I1, N, I, A, U) + ("IF" P[I] "THEN"
    TAMVEC(I1, N, I, A, V) "ELSE" A[I1,I] * V[I1])) / A[I,I];
    V[I]:= (V[I] - MATVEC(I1, N, I, A, V) - ("IF" P[I] "THEN"
    TAMVEC(I1, N, I, A, U) "ELSE" A[I1,I] * U[I1])) / A[I,I]
"END" BACKWARD;
NORMALISE: W:= 1 / SQRT(VECVEC(1, N, 0, U, U) +
    VECVEC(1, N, 0, V, V));
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" U[J]:= U[J] * W; V[J]:= V[J] * W "END";
COUNT:= COUNT + 1; "IF" W > TOL "THEN" "GOTO" FORWARD;
OUTM: EM[7]:= W; EM[9]:= COUNT
"END" COMVECHES;
"EOF"
    
```

SECTION 3.3.1.2.2

(JULY 1974)

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**BRIEF DESCRIPTION:**

THIS SECTION CONTAINS FIVE PROCEDURES FOR CALCULATING EIGENVALUES AND / OR EIGENVECTORS OF REAL MATRICES:

A) REAEIGVAL CALCULATES THE EIGENVALUES OF A MATRIX, PROVIDED THAT ALL EIGENVALUES ARE REAL,

B) REAEIG1 CALCULATES THE EIGENVALUES, PROVIDED THAT THEY ARE ALL REAL, AND THE EIGENVECTORS OF A MATRIX,

C) REAEIG3 CALCULATES THE EIGENVALUES, PROVIDED THAT THEY ARE ALL REAL, AND THE EIGENVECTORS OF A MATRIX,

D) COMEIGVAL CALCULATES THE EIGENVALUES OF A MATRIX,

E) COMEIG1 CALCULATES THE EIGENVALUES AND EIGENVECTORS OF A MATRIX.

**KEYWORDS:**

EIGENVALUES,  
EIGENVECTORS.

SUBSECTION: REAEIGVAL.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "INTEGER" "PROCEDURE" REAEIGVAL(A, N, EM, VAL); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, EM, VAL;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE MATRIX WHOSE EIGENVALUES ARE TO BE CALCULATED;  
 EXIT: THE ARRAY ELEMENTS ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EM[2], THE RELATIVE TOLERANCE USED FOR THE QR  
 ITERATION;  
 EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE  
 DATA TO BE GIVEN IN EM ARE:  
 EM[0] =  $\approx 14$ ,  
 EM[2] > EM[0] (E.G. EM[2] =  $\approx 13$ ),  
 EM[4] =  $10 * N$ ;  
 EXIT: EM[1], THE INFINITY NORM OF THE EQUILIBRATED MATRIX;  
 EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
 ELEMENTS NEGLECTED;  
 EM[5], THE NUMBER OF QR ITERATIONS PERFORMED;  
 IF THE ITERATION PROCESS IS NOT COMPLETED  
 WITHIN EM[4] ITERATIONS, THE VALUE EM[4] + 1  
 IS DELIVERED AND IN THIS CASE ONLY THE LAST  
 N - K ELEMENTS OF VAL ARE APPROXIMATE EIGEN-  
 VALUES OF THE GIVEN MATRIX, WHERE K IS  
 DELIVERED IN REAEIGVAL;

VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:N];  
 EXIT: THE EIGENVALUES OF THE GIVEN MATRIX ARE DELIVERED  
 IN MONOTONICALLY NONINCREASING ORDER;

MOREOVER;

REAEIGVAL DELIVERS 0, PROVIDED THAT THE PROCESS IS COMPLETED WITHIN  
 EM[4] ITERATIONS; OTHERWISE REAEIGVAL DELIVERS K, THE NUMBER OF  
 EIGENVALUES NOT CALCULATED.



PROCEDURES USED:

EQILBR = CP34173,  
TFMREAHES = CP34170,  
REAVLQRI = CP34180.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: 3N.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE GIVEN MATRIX IS EQUILIBRATED BY CALLING EQILBR (SEE SECTION 3.2.1.1.1) AND TRANSFORMED TO A SIMILAR UPPER-HESSSENBERG MATRIX BY CALLING TFMREAHES (SEE SECTION 3.2.1.2.1.2). THE EIGENVALUES ARE THEN CALCULATED BY CALLING REAVLQRI, WHICH USES SINGLE QR ITERATION (SEE SECTION 3.3.1.2.1).

THE PROCEDURE REAEIGVAL SHOULD BE USED ONLY IF ALL EIGENVALUES ARE REAL.

FOR FURTHER DETAILS SEE REFERENCES [1], [2] AND [3].

SUBSECTION: REAEIG1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"INTEGER" "PROCEDURE" REAEIG1(A, N, EM, VAL, VEC); "VALUE" N;  
"INTEGER" N; "ARRAY" A, EM, VAL, VEC;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;

"ARRAY" A[1:N,1:N];

ENTRY: THE MATRIX WHOSE EIGENVALUES AND EIGENVECTORS ARE TO BE CALCULATED;

EXIT: THE ARRAY ELEMENTS ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;

THE ORDER OF THE GIVEN MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:9];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
       EM[2], THE RELATIVE TOLERANCE USED FOR THE QR  
           ITERATION;  
       EM[4], THE MAXIMUM ALLOWED NUMBER OF QR  
           ITERATIONS;  
       EM[6], THE TOLERANCE USED FOR THE EIGENVECTORS;  
           FOR EACH EIGENVECTOR THE INVERSE ITERATION  
           ENDS IF THE EUCLIDEAN NORM OF THE RESIDUE  
           VECTOR IS SMALLER THAN EM[1] \* EM[6];  
       EM[8], THE MAXIMUM ALLOWED NUMBER OF INVERSE  
           ITERATIONS FOR THE CALCULATION OF EACH  
           EIGENVECTOR;  
       FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE  
       DATA TO BE GIVEN IN EM ARE:  
       EM[0] = "E-14,  
       EM[2] > EM[0] (E.G. EM[2] = "E-13),  
       EM[4] = 10 \* N,  
       EM[6] > EM[2] (E.G. EM[6] = "E-10),  
       EM[8] = 5;  
 EXIT: EM[1], THE INFINITY NORM OF THE EQUILIBRATED MATRIX;  
       EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
           ELEMENTS NEGLECTED;  
       EM[5], THE NUMBER OF QR ITERATIONS PERFORMED;  
           IF THE ITERATION PROCESS IS NOT COMPLETED  
           WITHIN EM[4] ITERATIONS, THE VALUE EM[4] + 1  
           IS DELIVERED AND IN THIS CASE ONLY THE LAST  
           N - K ELEMENTS OF VAL AND COLUMNS OF VEC ARE  
           APPROXIMATE EIGENVALUES AND EIGENVECTORS OF  
           THE GIVEN MATRIX, WHERE K IS DELIVERED IN  
           REAEIG1;  
       EM[7], THE MAXIMUM EUCLIDIAN NORM OF THE RESIDUES  
           OF THE CALCULATED EIGENVECTORS (OF THE TRANS-  
           FORMED MATRIX);  
       EM[9], THE LARGEST NUMBER OF INVERSE ITERATIONS  
           PERFORMED FOR THE CALCULATION OF SOME EIGEN-  
           VECTOR; IF, FOR SOME EIGENVECTOR THE  
           EUCLIDEAN NORM OF THE RESIDUE REMAINS  
           LARGER THAN EM[1] \* EM[6], THE VALUE  
           EM[8] + 1 IS DELIVERED; NEVERTHELESS THE  
           EIGENVECTORS MAY THEN VERY WELL BE USEFUL,  
           THIS SHOULD BE JUDGED FROM THE VALUE  
           DELIVERED IN EM[7] OR FROM SOME OTHER TEST;

VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:N];  
 EXIT: THE EIGENVALUES OF THE GIVEN MATRIX ARE DELIVERED  
       IN MONOTONICALLY DECREASING ORDER;

VEC: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC[1:N,1:N];  
 EXIT: THE CALCULATED EIGENVECTORS, CORRESPONDING TO THE  
       EIGENVALUES IN ARRAY VAL[1:N], ARE DELIVERED IN THE  
       COLUMNS OF ARRAY VEC;

MOREOVER:

REAEIG1 DELIVERS 0, PROVIDED THAT THE PROCESS IS COMPLETED WITHIN EM[4] ITERATIONS; OTHERWISE REAEIG1 DELIVERS K, THE NUMBER OF EIGENVALUES AND EIGENVECTORS NOT CALCULATED.

PROCEDURES USED:

EQILBR = CP34173,  
 TFMREAHES = CP34170,  
 BAKREAHES2 = CP34172,  
 BAKLBR = CP34174,  
 REAVALQRI = CP34180,  
 REAVECHES = CP34181,  
 REASCL = CP34183.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:  $N * N + 5N$ .

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

OPTIONS: F.

METHOD AND PERFORMANCE:

THE GIVEN MATRIX IS EQUILIBRATED BY CALLING EQILBR (SEE SECTION 3,2,1,1,1) AND TRANSFORMED TO A SIMILAR UPPER-HESSSENBERG MATRIX BY CALLING TFMREAHES (SEE SECTION 3,2,1,2,1,2). THE EIGENVALUES ARE THEN CALCULATED BY CALLING REAVALQRI, WHICH USES SINGLE QR ITERATION (SEE SECTION 3,3,1,2,1).

FURTHERMORE, TO FIND THE EIGENVECTORS WILKINSON'S DEVICE IS FIRST APPLIED [2, P.328 AND 628]. SUBSEQUENTLY THE EIGENVECTORS OF THE UPPER-HESSSENBERG MATRIX ARE CALCULATED BY CALLING REAVECHES, WHICH USES INVERSE ITERATION (SEE SECTION 3,3,1,2,1). THE CALCULATED VECTORS ARE THEN BACK-TRANSFORMED TO THE CORRESPONDING EIGENVECTORS OF THE GIVEN MATRIX BY CALLING BAKREAHES2 AND BAKLBR (SEE SECTIONS 3,2,1,2,1,2 AND 3,2,1,1,1). FINALLY THE APPROXIMATE EIGENVECTORS ARE NORMALIZED BY CALLING REASCL (SEE SECTION 1,1,9) SUCH THAT, IN EACH EIGENVECTOR, AN ELEMENT OF MAXIMUM ABSOLUTE VALUE EQUALS 1.

THE PROCEDURE REAEIG1 SHOULD BE USED ONLY IF ALL EIGENVALUES ARE REAL.

FOR FURTHER DETAILS SEE THE GIVEN REFERENCES.

SUBSECTION: REAEIG3.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "INTEGER" "PROCEDURE" REAEIG3(A, N, EM, VAL, VEC); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, EM, VAL, VEC;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE MATRIX WHOSE EIGENVALUES AND EIGENVECTORS ARE TO  
 BE CALCULATED;  
 EXIT: THE ARRAY ELEMENTS ARE ALTERED;  
 N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;  
 EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EM[2], THE RELATIVE TOLERANCE USED FOR THE QR  
 ITERATION;  
 EM[4], THE MAXIMUM ALLOWED NUMBER OF QR  
 ITERATIONS;  
 FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE  
 DATA TO BE GIVEN IN EM ARE:  
 EM[0] = ".14,  
 EM[2] > EM[0] (E.G. EM[2] = ".13),  
 EM[4] = 10 \* N;  
 EXIT: EM[1], THE INFINITY NORM OF THE EQUILIBRATED MATRIX;  
 EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
 ELEMENTS NEGLECTED;  
 EM[5], THE NUMBER OF QR ITERATIONS PERFORMED;  
 IF THE ITERATION PROCESS IS NOT COMPLETED  
 WITHIN EM[4] ITERATIONS, THE VALUE EM[4] + 1  
 IS DELIVERED. IN THIS CASE ONLY THE LAST  
 N \* K ELEMENTS OF VAL ARE APPROXIMATE  
 EIGENVALUES OF THE GIVEN MATRIX AND NO USEFUL  
 EIGENVECTORS ARE DELIVERED. THE VALUE K IS  
 DELIVERED IN REAEIG3;  
 VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:N];  
 EXIT: THE EIGENVALUES OF THE GIVEN MATRIX ARE DELIVERED;  
 VEC: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC[1:N,1:N];  
 EXIT: THE CALCULATED EIGENVECTORS, CORRESPONDING TO THE  
 EIGENVALUES IN ARRAY VAL[1:N], ARE DELIVERED IN THE  
 COLUMNS OF ARRAY VEC;

MOREOVER:

REAEIG3 DELIVERS 0, PROVIDED THAT THE PROCESS IS COMPLETED WITHIN  
 EM[4] ITERATIONS; OTHERWISE REAEIG3 DELIVERS K, THE NUMBER OF  
 EIGENVALUES NOT CALCULATED.

PROCEDURES USED:

EQILBR        = CP34173,  
 TFMREAHES    = CP34170,  
 BAKREAHES2   = CP34172,  
 BAKLBR        = CP34174,  
 REAGRI        = CP34186,  
 REASCL        = CP34183.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH: 4N.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE GIVEN MATRIX IS EQUILIBRATED BY CALLING EQILBR (SEE SECTION 3,2,1,1,1) AND TRANSFORMED TO A SIMILAR UPPER-HESSSENBERG MATRIX BY CALLING TFMREAHES (SEE SECTION 3,2,1,2,1,2). THE EIGENVALUES AND EIGENVECTORS OF THE UPPER-HESSSENBERG MATRIX ARE THEN CALCULATED BY CALLING REAGRI, WHICH USES SINGLE OR ITERATION FOR THE EIGENVALUES AND A DIRECT METHOD FOR THE EIGENVECTORS (SEE SECTION 3,3,1,2,1). FINALLY THE EIGENVECTORS OF THE UPPER-HESSSENBERG MATRIX ARE BACK-TRANSFORMED TO THE CORRESPONDING EIGENVECTORS OF THE GIVEN MATRIX BY CALLING BAKREAHES2 (SEE SECTION 3,1,2,1,2,1) AND NORMALIZED BY CALLING REASCL (SEE SECTION 1,1,9) SUCH THAT, IN EACH EIGENVECTOR, AN ELEMENT OF MAXIMUM ABSOLUTE VALUE EQUALS 1.

THE PROCEDURE REAEIG3 SHOULD BE USED ONLY IF ALL EIGENVALUES ARE REAL.

FOR FURTHER DETAILS SEE THE GIVEN REFERENCES.

SUBSECTION: COMEIGVAL.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "INTEGER" "PROCEDURE" COMEIGVAL(A, N, EM, RE, IM); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, EM, RE, IM;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE MATRIX WHOSE EIGENVALUES ARE TO BE CALCULATED;  
 EXIT: THE ARRAY ELEMENTS ARE ALTERED;

N:  
 <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM:  
 <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0], THE MACHINE PRECISION;  
 EM[2], THE RELATIVE TOLERANCE USED FOR THE QR  
 ITERATION;  
 EM[4], THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE  
 DATA TO BE GIVEN IN EM ARE:  
 EM[0] = "14,  
 EM[2] > EM[0] (E.G. EM[2] = "13),  
 EM[4] = 10 \* N;  
 EXIT: EM[1], THE INFINITY NORM OF THE EQUILIBRATED MATRIX;  
 EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
 ELEMENTS NEGLECTED;  
 EM[5], THE NUMBER OF QR ITERATIONS PERFORMED;  
 IF THE ITERATION PROCESS IS NOT COMPLETED  
 WITHIN EM[4] ITERATIONS, THE VALUE EM[4] + 1  
 IS DELIVERED AND IN THIS CASE ONLY THE LAST  
 N - K ELEMENTS OF RE AND IM ARE APPROXIMATE  
 EIGENVALUES OF THE GIVEN MATRIX, WHERE K IS  
 DELIVERED IN COMEIGVAL;

RE, IM: <ARRAY IDENTIFIER>;  
 "ARRAY" RE, IM[1:N];  
 EXIT: THE REAL AND IMAGINARY PARTS OF THE CALCULATED  
 EIGENVALUES OF THE GIVEN MATRIX ARE DELIVERED IN  
 ARRAY RE, IM[1:N], THE MEMBERS OF EACH NONREAL  
 COMPLEX CONJUGATE PAIR BEING CONSECUTIVE;

MOREOVER:

COMEIGVAL DELIVERS 0, PROVIDED THAT THE PROCESS IS COMPLETED WITHIN  
 EM[4] ITERATIONS; OTHERWISE COMEIGVAL DELIVERS K, THE NUMBER OF  
 EIGENVALUES NOT CALCULATED.

PROCEDURES USED:

EQILBR = CP34173,  
 TFMREAHES = CP34170,  
 COMVALQRI = CP34190.

REQUIRED CENTRAL MEMORY:  
 EXECUTION FIELD LENGTH: 3N.

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE GIVEN MATRIX IS EQUILIBRATED BY CALLING EQILBR (SEE SECTION 3.2.1.1.1) AND TRANSFORMED TO A SIMILAR UPPER-HESSSENBERG MATRIX BY CALLING TFMREAHES (SEE SECTION 3.2.1.2.1.2). THE EIGENVALUES ARE THEN CALCULATED BY CALLING COMVALQRI, WHICH USES DOUBLE QR ITERATION (SEE SECTION 3.3.1.2.1). FOR FURTHER DETAILS SEE REFERENCES [1], [2] AND [3].

SUBSECTION: COMEIG1.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"INTEGER" "PROCEDURE" COMEIG1(A, N, EM, RE, IM, VEC); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, EM, RE, IM, VEC;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;

"ARRAY" A[1:N,1:N];

ENTRY: THE MATRIX WHOSE EIGENVALUES AND EIGENVECTORS ARE TO BE CALCULATED;

EXIT: THE ARRAY ELEMENTS ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;

THE ORDER OF THE GIVEN MATRIX;

EM: <ARRAY IDENTIFIER>;

"ARRAY" EM[0:9];

ENTRY: EM[0], THE MACHINE PRECISION;

EM[2], THE RELATIVE TOLERANCE USED FOR THE QR ITERATION;

EM[4], THE MAXIMUM ALLOWED NUMBER OF QR ITERATIONS;

EM[6], THE TOLERANCE USED FOR THE EIGENVECTORS; FOR EACH EIGENVECTOR THE INVERSE ITERATION ENDS IF THE EUCLIDEAN NORM OF THE RESIDUE VECTOR IS SMALLER THAN EM[1] \* EM[6];

EM[8], THE MAXIMUM ALLOWED NUMBER OF INVERSE ITERATIONS FOR THE CALCULATION OF EACH EIGENVECTOR;

FOR THE CD CYBER 73-28 SUITABLE VALUES OF THE DATA TO BE GIVEN IN EM ARE:

EM[0] = "14,

EM[2] > EM[0] (E.G. EM[2] = "13),

EM[4] = 10 \* N,

EM[6] > EM[2] (E.G. EM[6] = "10),

EM[8] = 5;

EXIT: EM[1], THE INFINITY NORM OF THE EQUILIBRATED MATRIX;  
 EM[3], THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
 ELEMENTS NEGLECTED;  
 EM[5], THE NUMBER OF QR ITERATIONS PERFORMED;  
 IF THE ITERATION PROCESS IS NOT COMPLETED  
 WITHIN EM[4] ITERATIONS, THE VALUE EM[4] + 1  
 IS DELIVERED AND IN THIS CASE ONLY THE LAST  
 N - K ELEMENTS OF RE, IM AND COLUMNS OF VEC  
 ARE APPROXIMATE EIGENVALUES AND EIGENVECTORS  
 OF THE GIVEN MATRIX, WHERE K IS DELIVERED IN  
 COMEIG1;  
 EM[7], THE MAXIMUM EUCLIDIAN NORM OF THE RESIDUES  
 OF THE CALCULATED EIGENVECTORS (OF THE TRANS-  
 FORMED MATRIX);  
 EM[9], THE LARGEST NUMBER OF INVERSE ITERATIONS  
 PERFORMED FOR THE CALCULATION OF SOME EIGEN-  
 VECTOR; IF THE EUCLIDIAN NORM OF THE  
 RESIDUE FOR ONE OR MORE EIGENVECTORS REMAINS  
 LARGER THAN EM[1] \* EM[6], THE VALUE EM[8]+1  
 IS DELIVERED; NEVERTHELESS THE EIGENVECTORS  
 MAY THEN VERY WELL BE USEFUL, THIS SHOULD BE  
 JUDGED FROM THE VALUE DELIVERED IN EM[7] OR  
 FROM SOME OTHER TEST;

RE, IM: <ARRAY IDENTIFIER>;  
 "ARRAY" RE, IM[1:N];  
 EXIT: THE REAL AND IMAGINARY PARTS OF THE CALCULATED  
 EIGENVALUES OF THE GIVEN MATRIX ARE DELIVERED IN  
 ARRAY RE, IM[1:N], THE MEMBERS OF EACH NONREAL  
 COMPLEX CONJUGATE PAIR BEING CONSECUTIVE;

VEC: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC[1:N,1:N];  
 EXIT: THE CALCULATED EIGENVECTORS ARE DELIVERED IN THE  
 COLUMNS OF ARRAY VEC;  
 AN EIGENVECTOR, CORRESPONDING TO A REAL EIGENVALUE  
 GIVEN IN ARRAY RE, IS DELIVERED IN THE CORRESPONDING  
 COLUMN OF ARRAY VEC;  
 THE REAL AND IMAGINARY PART OF AN EIGENVECTOR,  
 CORRESPONDING TO THE FIRST MEMBER OF A NONREAL  
 COMPLEX CONJUGATE PAIR OF EIGENVALUES GIVEN IN THE  
 ARRAYS RE, IM, ARE DELIVERED IN THE TWO CONSECUTIVE  
 COLUMNS OF ARRAY VEC CORRESPONDING TO THIS PAIR (THE  
 EIGENVECTORS CORRESPONDING TO THE SECOND MEMBERS OF  
 NONREAL COMPLEX CONJUGATE PAIRS ARE NOT DELIVERED,  
 SINCE THEY ARE SIMPLY THE COMPLEX CONJUGATE OF THOSE  
 CORRESPONDING TO THE FIRST MEMBER OF SUCH PAIRS);

MOREOVER:  
 COMEIG1 DELIVERS 0, PROVIDED THAT THE PROCESS IS COMPLETED WITHIN  
 EM[4] ITERATIONS; OTHERWISE COMEIG1 DELIVERS K, THE NUMBER OF  
 EIGENVALUES AND EIGENVECTORS NOT CALCULATED.



PROCEDURES USED:

EQILBR       = CP34173,  
 TFMREAHES   = CP34170,  
 BAKREAHES2   = CP34172,  
 BAKLBR       = CP34174,  
 REAVECHES    = CP34181,  
 COMVALQRI    = CP34190,  
 COMVECHES    = CP34191,  
 COMSCL       = CP34193.

REQUIRED CENTRAL MEMORY:

EXECUTION FIELD LENGTH:  $N * N + 5N$ .

RUNNING TIME: ROUGHLY PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

THE GIVEN MATRIX IS EQUILIBRATED BY CALLING EQILBR (SEE SECTION 3,2,1,1,1) AND TRANSFORMED TO A SIMILAR UPPER-HESSSENBERG MATRIX BY CALLING TFMREAHES (SEE SECTION 3,2,1,2,1,2). THE EIGENVALUES ARE THEN CALCULATED BY CALLING COMVALQRI, WHICH USES DOUBLE QR ITERATION (SEE SECTION 3,3,1,2,1).

FURTHERMORE, TO FIND THE EIGENVECTORS WILKINSON'S DEVICE IS FIRST APPLIED [2, P.328 AND 628]. SUBSEQUENTLY THE EIGENVECTORS OF THE UPPER-HESSSENBERG MATRIX ARE COMPUTED BY CALLING REAVECHES FOR THE REAL EIGENVALUES AND COMVECHES FOR THE OTHERS (SECTION 3,3,1,2,1.) THE COMPUTED VECTORS ARE THEN BACK-TRANSFORMED TO THE CORRESPONDING EIGENVECTORS OF THE GIVEN MATRIX BY CALLING BAKREAHES2 AND BAKLBR (SEE SECTIONS 3,2,1,2,1,2 AND 3,2,1,1,1). FINALLY THE APPROXIMATE EIGENVECTORS ARE NORMALIZED BY CALLING COMSCL (SEE SECTION 1,1,9) SUCH THAT, IN EACH EIGENVECTOR, AN ELEMENT OF MAXIMUM MODULUS EQUALS 1.

FOR FURTHER DETAILS SEE THE GIVEN REFERENCES.

REFERENCES:

- [1]. T.J. DEKKER AND W. HOFFMANN.  
ALGOL 60 PROCEDURES IN NUMERICAL ALGEBRA, PART 2,  
MC TRACT 23, 1968, MATH. CENTR., AMSTERDAM.
- [2]. J.H. WILKINSON.  
THE ALGEBRAIC EIGENVALUE PROBLEM.  
CLARENDON PRESS, OXFORD, 1965.
- [3]. J.G. FRANCIS.  
THE QR TRANSFORMATION, PARTS 1 AND 2.  
COMP. J. 4 (1961), 265 - 271 AND 332 - 345.
- [4]. J.M. VARAH.  
EIGENVECTORS OF A REAL MATRIX BY INVERSE ITERATION.  
STANFORD UNIVERSITY, TECH. REP. NO. CS 34, 1966.

EXAMPLE OF USE:

IN THIS SECTION WE ONLY GIVE AN EXAMPLE OF USE OF THE PROCEDURES REAEIG3 AND COMEIGVAL, BECAUSE A CALL OF THE OTHER PROCEDURES IS ALMOST SIMILAR.

THE EIGENVALUES AND CORRESPONDING EIGENVECTORS OF A MATRIX, STORED IN ARRAY A, WITH  $A[I,J] := \text{"IF" } I = J \text{ "THEN" } 1 \text{ "ELSE" } 1 / (I + J - 1)$ , MAY BE OBTAINED BY THE PROCEDURE REAEIG3 IN THE FOLLOWING PROGRAM:

```
"BEGIN" "INTEGER" I, J, M;
  "ARRAY" A, VEC[1:4,1:4], EM[0:5], VAL[1:4];
  "INTEGER" "PROCEDURE" REAEIG3(A, N, EM, VAL, VEC);
  "CODE" 34187;

  "FOR" I:= 1, 2, 3, 4 "DO" "FOR" J:= 1, 2, 3, 4 "DO"
  A[I,J]:= "IF" I = J "THEN" 1 "ELSE" 1 / ( I + J - 1);
  EM[0]:= "-14; EM[2]:= "-13; EM[4]:= 40;
  M:= REAEIG3(A, 4, EM, VAL, VEC);
  OUTPUT(61, "(D, /)", M);
  "FOR" I:= M + 1 "STEP" 1 "UNTIL" 4 "DO"
  OUTPUT(61, "(/, 2(+.13D"+2D, 2B), /, 3(21B, +.13D"+2D, /))",
  VAL[I], VEC[1,I], VEC[2,I], VEC[3,I], VEC[4,I]);
  OUTPUT(61, "(/, 2(.2D"+2D, /), ZD)", EM[1], EM[3], EM[5])
"END"
```

THE PROGRAM DELIVERS (THE RESULTS ARE CORRECT UP TO TWELVE DIGITS):

THE NUMBER OF NOT CALCULATED EIGENVALUES: 0

THE EIGENVALUES AND CORRESPONDING EIGENVECTORS:

+ .1886632138548"+01	+ .10000000000000"+01
	+ .3942239850770"+00
	+ .2773202862566"+00
	+ .2150878672143"+00
- .1980145931103"+00	+ .10000000000000"+01
	- .7388484093937"+00
	- .3116238593839"+00
	- .1475423243327"+00
- .1228293686543"-01	- .4634736456357"+00
	+ .10000000000000"+01
	- .1542548002737"+00
	- .3765787365625"+00
- .1441323817331"-03	+ .1095712655340"+00
	- .6208405341138"+00
	+ .10000000000000"+01
	- .4887465241876"+00

EM[1] = .40"+01  
 EM[3] = .15"-14  
 EM[5] = 5 ,

THE COMPLEX EIGENVALUES OF A MATRIX STORED IN ARRAY A WITH  $N = 3$  AND THE ROWS  $(8, -1, -5)$ ,  $(-4, 4, -2)$  AND  $(18, -5, -7)$ , MAY BE OBTAINED BY THE PROCEDURE COMEIGVAL IN THE FOLLOWING PROGRAM:

```
"BEGIN" "INTEGER" I, M;
  "ARRAY" A[1:3,1:3], EM[0:5], RE, IM[1:3];
  "INTEGER" "PROCEDURE" COMEIGVAL(A, N, EM, RE, IM);
  "CODE" 34192;

  EM[0] := "-14; EM[2] := "-13; EM[4] := 30;
  A[1,1] := 8; A[1,2] := -1; A[1,3] := -5;
  A[2,1] := -4; A[2,2] := 4; A[2,3] := -2;
  A[3,1] := 18; A[3,2] := -5; A[3,3] := -7;
  M := COMEIGVAL(A, 3, EM, RE, IM);
  OUTPUT(61, "("D, /)", M);
  "FOR" I := M + 1 "STEP" 1 "UNTIL" 3 "DO"
  OUTPUT(61, "("2(+,13D"+2D, 2B), /)", RE[I], IM[I]);
  OUTPUT(61, "("/, 2(,2D"+2D, /), ZD)", EM[1], EM[3], EM[5])
"END"
```

THE PROGRAM DELIVERS(THE RESULTS ARE CORRECT UP TO TWELVE DIGITS):

THE NUMBER OF NOT CALCULATED EIGENVALUES: 0

THE EIGENVALUES:  $+ .2000000000000000^{+01}$   $+ .4000000000000000^{+01}$   
 $+ .2000000000000000^{+01}$   $+ .4000000000000000^{+01}$   
 $+ .9999999999999998^{+00}$   $+ .0000000000000000^{+00}$

THE ARRAY EM: EM[1] =  $.30^{+02}$   
 EM[3] =  $.78^{-17}$   
 EM[5] = 6 .

SOURCE TEXTS:

```
"CODE" 34182;
"COMMENT" MCA 2412;
"INTEGER" "PROCEDURE" REAEIGVAL(A, N, EM, VAL); "VALUE" N;
"INTEGER" N; "ARRAY" A, EM, VAL;
"BEGIN" "INTEGER" I, J; "REAL" R;
  "ARRAY" D[1:N]; "INTEGER" "ARRAY" INT, INTO[1:N];

  "PROCEDURE" TFMREAHES(A, N, EM, INT); "CODE" 34170;
  "PROCEDURE" EQILBR(A, N, EM, D, INT); "CODE" 34173;
  "INTEGER" "PROCEDURE" REAVALQRI(A, N, EM, VAL); "CODE" 34180;

  EQILBR(A, N, EM, D, INTO); TFMREAHES(A, N, EM, INT);
  J := REAEIGVAL := REAVALQRI(A, N, EM, VAL);
  "FOR" I := J + 1 "STEP" 1 "UNTIL" N "DO"
  "FOR" J := I + 1 "STEP" 1 "UNTIL" N "DO"
  "BEGIN" "IF" VAL[J] > VAL[I] "THEN"
    "BEGIN" R := VAL[I]; VAL[I] := VAL[J]; VAL[J] := R "END"
  "END"
"END" REAEIGVAL;
"EOF"
```

```

"CODE" 34184;
"COMMENT" MCA 2414;
"INTEGER" "PROCEDURE" REAEIG1(A, N, EM, VAL, VEC); "VALUE" N;
"INTEGER" N; "ARRAY" A, EM, VAL, VEC;
"BEGIN" "INTEGER" I, K, MAX, J, L;
      "REAL" RESIDU, R, MACHTOL;
      "ARRAY" D, V[1:N], B[1:N,1:N];
      "INTEGER" "ARRAY" INT, INTO[1:N];

      "PROCEDURE" TFMREAHES(A, N, EM, INT); "CODE" 34170;
      "PROCEDURE" BAKREAHES2(A, N, N1, N2, INT, VEC); "CODE" 34172;
      "PROCEDURE" EQILBR(A, N, EM, D, INT); "CODE" 34173;
      "PROCEDURE" BAKLBR(N, N1, N2, D, INT, VEC); "CODE" 34174;
      "INTEGER" "PROCEDURE" REAVALORI(A, N, EM, VAL); "CODE" 34180;
      "PROCEDURE" REAVECHES(A, N, LAMBDA, EM, V); "CODE" 34181;
      "PROCEDURE" REASCL(A, N, N1, N2); "CODE" 34183;

      RESIDU := 0; MAX := 0; EQILBR(A, N, EM, D, INTO);
      TFMREAHES(A, N, EM, INT);
      "FOR" I := 1 "STEP" 1 "UNTIL" N "DO"
      "FOR" J := ("IF" I = 1 "THEN" 1 "ELSE" I + 1)
      "STEP" 1 "UNTIL" N "DO" B[I,J] := A[I,J];
      K := REAEIG1 := REAVALORI(B, N, EM, VAL);
      "FOR" I := K + 1 "STEP" 1 "UNTIL" N "DO"
      "FOR" J := I + 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" "IF" VAL[J] > VAL[I] "THEN"
          "BEGIN" R := VAL[I]; VAL[I] := VAL[J]; VAL[J] := R "END"
      "END";
      MACHTOL := EM[0] * EM[1];
      "FOR" L := K + 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" "IF" L > 1 "THEN"
          "BEGIN" "IF" VAL[L = 1] = VAL[L] < MACHTOL "THEN"
              VAL[L] := VAL[L = 1] * MACHTOL
          "END";
          "FOR" I := 1 "STEP" 1 "UNTIL" N "DO"
          "FOR" J := ("IF" I = 1 "THEN" 1 "ELSE" I + 1)
          "STEP" 1 "UNTIL" N "DO" B[I,J] := A[I,J];
          REAVECHES(B, N, VAL[L], EM, V);
          "IF" EM[7] > RESIDU "THEN" RESIDU := EM[7];
          "IF" EM[9] > MAX "THEN" MAX := EM[9];
          "FOR" J := 1 "STEP" 1 "UNTIL" N "DO" VEC[J,L] := V[J]
      "END";
      EM[7] := RESIDU; EM[9] := MAX;
      BAKREAHES2(A, N, K + 1, N, INT, VEC);
      BAKLBR(N, K + 1, N, D, INTO, VEC);
      REASCL(VEC, N, K + 1, N)
"END" REAEIG1;
"EOP"

```

```

"CODE" 34187;
"COMMENT" MCA 2417;
"INTEGER" "PROCEDURE" REAEIG3(A, N, EM, VAL, VEC); "VALUE" N;
"INTEGER" N; "ARRAY" A, EM, VAL, VEC;
"BEGIN" "INTEGER" I; "REAL" S;
      "INTEGER" "ARRAY" INT, INTO[1:N]; "ARRAY" D[1:N];

      "PROCEDURE" TFMREAHES(A, N, EM, INT); "CODE" 34170;
      "PROCEDURE" BAKREAHES2(A, N, N1, N2, INT, VEC); "CODE" 34172;
      "PROCEDURE" EQILBR(A, N, EM, D, INT); "CODE" 34173;
      "PROCEDURE" BAKLBR(N, N1, N2, D, INT, VEC); "CODE" 34174;
      "PROCEDURE" REASCL(A, N, N1, N2); "CODE" 34183;
      "INTEGER" "PROCEDURE" REAQRI(A, N, EM, VAL, VEC); "CODE" 34186;

      EQILBR(A, N, EM, D, INTO); TFMREAHES(A, N, EM, INT);
      I:= REAEIG3; REAQRI(A, N, EM, VAL, VEC);
      "IF" I = 0 "THEN"
      "BEGIN" BAKREAHES2(A, N, 1, N, INT, VEC);
            BAKLBR(N, 1, N, D, INTO, VEC); REASCL(VEC, N, 1, N)
      "END"
"END" REAEIG3;
"EOF"

"CODE" 34192;
"COMMENT" MCA 2422;
"INTEGER" "PROCEDURE" COMEIGVAL(A, N, EM, RE, IM); "VALUE" N;
"INTEGER" N; "ARRAY" A, EM, RE, IM;
"BEGIN" "INTEGER" "ARRAY" INT, INTO[1:N];
      "ARRAY" D[1:N];

      "PROCEDURE" EQILBR(A, N, EM, D, INT); "CODE" 34173;
      "PROCEDURE" TFMREAHES(A, N, EM, INT); "CODE" 34170;
      "INTEGER" "PROCEDURE" COMVALQRI(A, N, EM, RE, IM);
      "CODE" 34190;

      EQILBR(A, N, EM, D, INTO); TFMREAHES(A, N, EM, INT);
      COMEIGVAL:= COMVALQRI(A, N, EM, RE, IM)
"END" COMEIGVAL;
"EOF"

```

```

"CODE" 34194;
"COMMENT" MCA 2424;
"INTEGER" "PROCEDURE" COMEIG1(A, N, EM, RE, IM, VEC);
"VALUE" N; "INTEGER" N;
"ARRAY" A, EM, RE, IM, VEC;
"BEGIN" "INTEGER" I, J, K, PJ, ITT;
"REAL" X, Y, MAX, NEPS;
"ARRAY" AB[1:N,1:N], D, U, V[1:N];
"INTEGER" "ARRAY" INT, INTO[1:N];

"PROCEDURE" TRANSFER;
"BEGIN" "INTEGER" I, J;
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"FOR" J:= ("IF" I = 1 "THEN" 1 "ELSE" I - 1) "STEP" 1
"UNTIL" N "DO" AB[I,J]:= A[I,J]
"END" TRANSFER;

"PROCEDURE" EGILBR(A, N, EM, D, INT); "CODE" 34173;
"PROCEDURE" TFMREAHES(A, N, EM, INT); "CODE" 34170;
"PROCEDURE" BAKREAHES2(A, N, N1, N2, INT, VEC); "CODE" 34172;
"PROCEDURE" BAKLBR(N, N1, N2, D, INT, VEC); "CODE" 34174;
"PROCEDURE" REAVECHES(A, N, LAMBDA, EM, V); "CODE" 34181;
"PROCEDURE" COMSCL(A, N, N1, N2, IM); "CODE" 34193;
"INTEGER" "PROCEDURE" COMVALQRI(A, N, EM, RE, IM);
"CODE" 34190;
"PROCEDURE" COMVECHES(A, N, LAMBDA, MU, EM, U, V);
"CODE" 34191;

EQILBR(A, N, EM, D, INTO); TFMREAHES(A, N, EM, INT); TRANSFER;
K:= COMEIG1:= COMVALQRI(AB, N, EM, RE, IM);
NEPS:= EM[0] * EM[1]; MAX:= 0; ITT:= 0;
"FOR" I:= K + 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" X:= RE[I]; Y:= IM[I]; PJ:= 0;
AGAIN: "FOR" J:= K + 1 "STEP" 1 "UNTIL" I + 1 "DO"
"BEGIN" "IF" ((X = RE[J]) ** 2 +
(Y = IM[J]) ** 2 <= NEPS ** 2) "THEN"
"BEGIN" "IF" PJ = J "THEN" NEPS:= EM[2] * EM[1]
"ELSE" PJ:= J; X:= X + 2 * NEPS; "GOTO" AGAIN
"END"
"END";
RE[I]:= X; TRANSFER; "IF" Y = 0 "THEN"
"BEGIN" COMVECHES(AB, N, RE[I], IM[I], EM, U, V);
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO" VEC[J,I]:= U[J];
I:= I + 1; RE[I]:= X
"END"
"ELSE" REAVECHES(AB, N, X, EM, V);
"FOR" J:= 1 "STEP" 1 "UNTIL" N "DO" VEC[J,I]:= V[J];
"IF" EM[7] > MAX "THEN" MAX:= EM[7];
ITT:= "IF" ITT > EM[9] "THEN" ITT "ELSE" EM[9]
"END";
EM[7]:= MAX; EM[9]:= ITT; BAKREAHES2(A, N, K + 1, N, INT, VEC);
BAKLBR(N, K + 1, N, D, INTO, VEC); COMSCL(VEC, N, K + 1, N, IM)
"END" COMEIG1;
"EOP"

```

SECTION 3.3.2.1

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## BRIEF DESCRIPTION:

THIS SECTION CONTAINS FOUR PROCEDURES FOR CALCULATING THE EIGENVALUES OR THE EIGENVALUES AND EIGENVECTORS OF COMPLEX HERMITIAN MATRICES.

EIGVALHRM CALCULATES THE EIGENVALUES OF A HERMITIAN MATRIX.

EIGHRM CALCULATES THE EIGENVALUES AND EIGENVECTORS OF A HERMITIAN MATRIX.

GRIVALHRM CALCULATES THE EIGENVALUES OF A HERMITIAN MATRIX.

QRIHRM CALCULATES THE EIGENVALUES AND EIGENVECTORS OF A HERMITIAN MATRIX.

WHEN A SMALL NUMBER OF EIGENVALUES OR EIGENVALUES AND EIGENVECTORS IS REQUIRED, THE USE OF EIGVALHRM OR EIGHRM IS RECOMMENDED; WHEN MORE THAN, SAY, 25 PERCENT OF THE EIGENSYSTEM IS REQUIRED, THE PROCEDURES GRIVALHRM OR QRIHRM ARE TO BE USED.

SUBSECTION: EIGVALHRM.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE READS ;  
 "PROCEDURE" EIGVALHRM(A, N, NUMVAL, VAL, EM); "VALUE" N, NUMVAL;  
 "INTEGER" N, NUMVAL; "ARRAY" A, VAL, EM;

THE MEANING OF THE FORMAL PARAMETERS IS :

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE REAL PART OF THE UPPER TRIANGLE OF THE  
 HERMITIAN MATRIX MUST BE GIVEN IN THE UPPER  
 TRIANGULAR PART OF A (THE ELEMENTS A[I,J], I<=J);  
 THE IMAGINARY PART OF THE STRICT LOWER TRIANGLE  
 OF THE HERMITIAN MATRIX MUST BE GIVEN IN THE  
 STRICT LOWER PART OF A (THE ELEMENTS A[I,J], I>J);  
 THE ELEMENTS OF A ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

NUMVAL: <ARITHMETIC EXPRESSION>;  
 EIGVALHRM CALCULATES THE LARGEST NUMVAL EIGENVALUES OF  
 THE HERMITIAN MATRIX;

VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:NUMVAL];  
 EXIT:  
 IN ARRAY VAL THE LARGEST NUMVAL EIGENVALUES ARE  
 DELIVERED IN MONOTONICALLY NONINCREASING ORDER;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:3];  
 ENTRY:  
 EM[0]: THE MACHINE PRECISION;  
 EM[2]: THE RELATIVE TOLERANCE FOR THE EIGENVALUES;  
 MORE PRECISELY; THE TOLERANCE FOR EACH EIGENVALUE  
 LAMBDA, IS ABS(LAMBDA)\*EM[2]+EM[1]\*EM[0];  
 EXIT:  
 EM[1]: AN ESTIMATE OF A NORM OF THE ORIGINAL MATRIX;  
 EM[3]: THE NUMBER OF ITERATIONS PERFORMED.

PROCEDURES USED:

HSHHRMTRIVAL = CP34364,  
 VALSYMTRI = CP34151.

REQUIRED CENTRAL MEMORY:

TWO AUXILIARY ARRAYS OF ORDER N AND N - 1 RESPECTIVELY ARE DECLARED

RUNNING TIME: PROPORTIONAL TO N CUBED.



LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE EIGHRM (THIS SECTION).

EXAMPLE OF USE: SEE EIGHRM (THIS SECTION).

SUBSECTION: EIGHRM.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE READS :  
 "PROCEDURE" EIGHRM(A, N, NUMVAL, VAL, VECR, VECI, EM);  
 "VALUE" N, NUMVAL; "INTEGER" N, NUMVAL;  
 "ARRAY" A, VAL, VECR, VECI, EM;

THE MEANING OF THE FORMAL PARAMETERS IS :

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE REAL PART OF THE UPPER TRIANGLE OF THE  
 HERMITIAN MATRIX MUST BE GIVEN IN THE UPPER  
 TRIANGULAR PART OF A (THE ELEMENTS A[I,J], I<=J);  
 THE IMAGINARY PART OF THE STRICT LOWER TRIANGLE  
 OF THE HERMITIAN MATRIX MUST BE GIVEN IN THE  
 STRICT LOWER PART OF A (THE ELEMENTS A[I,J], I>J);  
 THE ELEMENTS OF A ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

NUMVAL: <ARITHMETIC EXPRESSION>;  
 EIGHRM CALCULATES THE LARGEST NUMVAL EIGENVALUES OF THE  
 HERMITIAN MATRIX;

VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:NUMVAL];  
 EXIT;  
 IN ARRAY VAL THE LARGEST NUMVAL EIGENVALUES ARE  
 DELIVERED IN MONOTONICALLY NONINCREASING ORDER;

VECR, VECI: <ARRAY IDENTIFIER>;  
 "ARRAY" VECR, VECI[1:N,1:NUMVAL];  
 EXIT;  
 THE CALCULATED EIGENVECTORS;  
 THE COMPLEX EIGENVECTOR WITH REAL PART VECR[1:N,I] AND  
 IMAGINARY PART VECI[1:N,I] CORRESPONDS TO THE EIGENVALUE  
 VAL[I], I=1,...,NUMVAL;

EM:            <ARRAY IDENTIFIER>  
 "ARRAY" EM(019);  
 ENTRY;  
 EM(0): THE MACHINE PRECISION;  
 EM(2): THE RELATIVE TOLERANCE FOR THE EIGENVALUES;  
       MORE PRECISELY; THE TOLERANCE FOR EACH EIGENVALUE  
       LAMBDA, IS  $ABS(LAMBDA) * EM(2) + EM(1) * EM(0)$ ;  
 EM(4): THE ORTHOGONALIZATION PARAMETER (E.G. .01);  
 EM(6): THE TOLERANCE FOR THE EIGENVECTORS;  
 EM(8): THE MAXIMUM NUMBER OF INVERSE ITERATIONS ALLOWED  
       FOR THE CALCULATION OF EACH EIGENVECTOR;  
 EXIT;  
 EM(1): AN ESTIMATE OF A NORM OF THE ORIGINAL MATRIX;  
 EM(3): THE NUMBER OF ITERATIONS PERFORMED;  
 EM(5): THE NUMBER OF EIGENVECTORS INVOLVED IN THE LAST  
       GRAM-SCHMIDT ORTHOGONALIZATION;  
 EM(7): THE MAXIMUM EUCLIDEAN NORM OF THE RESIDUES OF THE  
       CALCULATED EIGENVECTORS;  
 EM(9): THE LARGEST NUMBER OF INVERSE ITERATIONS  
       PERFORMED FOR THE CALCULATION OF SOME  
       EIGENVECTOR; IF, HOWEVER, FOR SOME CALCULATED  
       EIGENVECTOR, THE EUCLIDEAN NORM OF THE RESIDUES  
       REMAINS GREATER THAN  $EM(1) * EM(6)$ , THEN  
        $EM(9) := EM(8) + 1$ .

PROCEDURES USED:

HSHRMTRI = CP34363,  
 VALSYMTRI = CP34151,  
 VECSYMTRI = CP34152,  
 BAKHRMTRI = CP34365.

REQUIRED CENTRAL MEMORY:

THREE AUXILIARY ARRAYS OF ORDER  $N-1$  AND TWO OF ORDER  $N$  ARE DECLARED

RUNNING TIME: PROPORTIONAL TO  $N$  CUBED.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE GRIHRM (THIS SECTION).

## EXAMPLE OF USE:

LET EIGHRM CALCULATE THE LARGEST EIGENVALUE AND THE CORRESPONDING EIGENVECTOR OF THE FOLLOWING MATRIX:

(SEE GREGORY AND KARNEY, CHAPTER 6, EXAMPLE 6,6)

$$\begin{matrix} 3 & 1 & 0 & +2I \\ 1 & 3 & -2I & 0 \\ 0 & +2I & 1 & 1 \\ -2I & 0 & 1 & 1 \end{matrix}$$

THE EIGENVECTORS ARE NORMALIZED BY THE PROCEDURE SCLCOM (SEE SECTION 1,2,11. ),

```
"BEGIN"
"COMMENT" GREGORY AND KARNEY, CHAPTER 6, EXAMPLE 6,6;
"PROCEDURE" SCLCOM(AR, AI, N, N1, N2); "CODE" 34360;
"PROCEDURE" INIMAT(LR, UR, LC, UC, A, X); "CODE" 31011;
"PROCEDURE" EIGHRM(A, N, NUMVAL, VAL, VECR, VECI, EM); "CODE" 34369;
"REAL" "ARRAY" A[1:4, 1:4], VAL[1:1], VECR, VECI[1:4, 1:1], EM[0:9];
"INTEGER" I;
INIMAT(1, 4, 1, 4, A, 0);
A[1, 1] := A[2, 2] := 3;
A[1, 2] := A[3, 3] := A[3, 4] := A[4, 4] := 1;
A[3, 2] := 2; A[4, 1] := -2;
EM[0] := 5; EM[2] := -12;
EM[4] := 0; EM[6] := -10; EM[8] := 5;
EIGHRM(A, 4, 1, VAL, VECR, VECI, EM);
SCLCOM(VECR, VECI, 4, 1, 1);
OUTPUT(61, "(" ("LARGEST EIGENVALUE: ") ", N/" " ", VAL[1]);
OUTPUT(61, "(" ("CORRESPONDING EIGENVECTOR: ") ", "/" " " ");
"FOR" I:=1, 2, 3, 4 "DO"
OUTPUT(61, "(" "+D, D, +D, DDD, "(" "*I" " ", "/" " " ", VECR[I, 1], VECI[I, 1]);
"FOR" I:=1, 3, 5, 7, 9 "DO"
OUTPUT(61, "(" "/" " "(" "EM[" " " ", D, "(" "]: " " ", +D, DDD "+DD" " " ", I, EM[I]);
"END"
```

## DELIVERS:

LARGEST EIGENVALUE: +4.8284271247462"000

CORRESPONDING EIGENVECTOR:

+1, 0+0, 000\*I

+1, 0+0, 000\*I

+0, 0+0, 414\*I

+0, 0+0, 414\*I

EM[1]: +6, 000"+00

EM[3]: +1, 800"+01

EM[5]: +1, 000"+00

EM[7]: +5, 303"-14

EM[9]: +1, 000"+00

SUBSECTION: QRIVALHRM.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE READS :  
 "INTEGER" "PROCEDURE" QRIVALHRM(A, N, VAL, EM); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, VAL, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A(1:N,1:N);  
 ENTRY: THE REAL PART OF THE UPPER TRIANGLE OF THE  
 HERMITIAN MATRIX MUST BE GIVEN IN THE UPPER  
 TRIANGULAR PART OF A (THE ELEMENTS A(I,J), I<=J);  
 THE IMAGINARY PART OF THE STRICT LOWER TRIANGLE  
 OF THE HERMITIAN MATRIX MUST BE GIVEN IN THE  
 STRICT LOWER PART OF A (THE ELEMENTS A(I,J), I>J);

N: THE ELEMENTS OF A ARE ALTERED;  
 <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL(1:N);

EM: EXIT;  
 THE CALCULATED EIGENVALUES;  
 <ARRAY IDENTIFIER>;  
 "ARRAY" EM(0:5);  
 ENTRY:  
 EM(0): THE MACHINE PRECISION;  
 EM(2): THE RELATIVE TOLERANCE FOR THE QR ITERATION;  
 EM(4): THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 EXIT:  
 EM(1): AN ESTIMATE OF A NORM OF THE ORIGINAL MATRIX;  
 EM(3): THE MAXIMUM ABSOLUTE VALUE OF THE CDDIAGONAL  
 ELEMENTS NEGLECTED;  
 EM(5): THE NUMBER OF ITERATIONS PERFORMED;  
 EM(5) = EM(4)+1 IN THE CASE QRIVALHRM=0;

QRIVALHRM=0, PROVIDED THE QR ITERATION IS COMPLETED WITHIN EM(4)  
 ITERATIONS; OTHERWISE, QRIVALHRM=THE NUMBER OF EIGENVALUES, K, NOT  
 CALCULATED AND ONLY THE LAST N-K ELEMENTS OF VAL ARE APPROXIMATE  
 EIGENVALUES OF THE ORIGINAL HERMITEAN MATRIX,

PROCEDURES USED:

HSHHRMTRIVAL = CP34364,  
 QRIVALSYMTRI = CP34160.

REQUIRED CENTRAL MEMORY:

TWO AUXILIARY ARRAYS OF ORDER N ARE DECLARED,

RUNNING TIME: PROPORTIONAL TO N CUBED,

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE QRIHRM (THIS SECTION).

EXAMPLE OF USE: SEE QRIHRM (THIS SECTION).

SUBSECTION: QRIHRM.

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE READS :  
 "INTEGER" "PROCEDURE" QRIHRM(A, N, VAL, VR, VI, EM); "VALUE" N;  
 "INTEGER" N; "ARRAY" A, VAL, VR, VI, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;  
 "ARRAY" A[1:N,1:N];  
 ENTRY: THE REAL PART OF THE UPPER TRIANGLE OF THE  
 HERMITIAN MATRIX MUST BE GIVEN IN THE UPPER  
 TRIANGULAR PART OF A (THE ELEMENTS A[I,J], I<=J);  
 THE IMAGINARY PART OF THE STRICT LOWER TRIANGLE  
 OF THE HERMITIAN MATRIX MUST BE GIVEN IN THE  
 STRICT LOWER PART OF A (THE ELEMENTS A[I,J], I>J);  
 THE ELEMENTS OF A ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

VAL: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL[1:N];  
 EXIT:

VR, VI: THE CALCULATED EIGENVALUES;  
 <ARRAY IDENTIFIER>;  
 "ARRAY" VR, VI[1:N,1:N];  
 EXIT:

EM: THE CALCULATED EIGENVECTORS;  
 THE COMPLEX EIGENVECTOR WITH REAL PART VR[1:N,I] AND  
 IMAGINARY PART VI[1:N,I] CORRESPONDS TO THE EIGENVALUE  
 VAL[I], I=1,...,N;  
 <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY:

EM[0]: THE MACHINE PRECISION;  
 EM[2]: THE RELATIVE TOLERANCE FOR THE QR ITERATION;  
 (E.G. THE MACHINE PRECISION);  
 EM[4]: THE MAXIMUM ALLOWED NUMBER OF ITERATIONS;  
 (E.G. 10 \* N);  
 EXIT:

EM[1]: AN ESTIMATE OF A NORM OF THE ORIGINAL MATRIX;  
 EM[3]: THE MAXIMUM ABSOLUTE VALUE OF THE CODIAGONAL  
 ELEMENTS NEGLECTED;  
 EM[5]: THE NUMBER OF ITERATIONS PERFORMED;  
 EM[5]=EM[4]+1 IN THE CASE QRIHRM=0;

QRIHRM=0, PROVIDED THE PROCESS IS COMPLETED WITHIN EM[4] ITERATIONS; OTHERWISE, QRIHRM= THE NUMBER OF EIGENVALUES, K, NOT CALCULATED AND ONLY THE LAST N-K ELEMENTS OF VAL ARE APPROXIMATE EIGENVALUES AND THE COLUMNS OF THE ARRAYS VR, VI[1:N, N-K:N] ARE APPROXIMATE EIGENVECTORS OF THE ORIGINAL HERMITEAN MATRIX ,

PROCEDURES USED:

HSHHRMTRI = CP34363,  
 GRISYMTRI = CP34161,  
 BAKHRMTRI = CP34365.

REQUIRED CENTRAL MEMORY:

TWO AUXILIARY ARRAYS OF ORDER N - 1 AND TWO OF ORDER N ARE DECLARED

RUNNING TIME: PROPORTIONAL TO N CUBED.

LANGUAGE: ALGOL 60.

THE FOLLOWING HOLDS FOR THE FOUR PROCEDURES OF THIS SECTION:

METHOD AND PERFORMANCE:

FOR THE TRANSFORMATION OF THE GIVEN HERMITIAN MATRIX INTO A REAL SYMMETRIC TRIDIAGONAL MATRIX, AND FOR THE CORRESPONDING BACK TRANSFORMATION, PROCEDURES OF SECTION 3.2.1.2,2.1. ARE USED. FOR THE CALCULATION OF THE EIGENVALUES AND EIGENVECTORS OF THE RESULTING SYMMETRIC TRIDIAGONAL MATRIX, PROCEDURES OF SECTION 3.3.1.1.1. ARE USED.

EXAMPLE OF USE:

QRIHRM CALCULATES THE EIGENVALUES AND EIGENVECTORS OF THE FOLLOWING MATRIX:  
 (SEE GREGORY AND KARNEY, CHAPTER 6, EXAMPLE 6,6)

3	1	0	+2I
1	3	-2I	0
0	+2I	1	1
-2I	0	1	1

THE EIGENVECTORS ARE NORMALIZED BY THE PROCEDURE SCLCOM (SEE SECTION 1,2,11. ). ONLY THE EIGENVECTORS CORRESPONDING TO VAL[2] AND VAL[3] ARE PRINTED BY THE FOLLOWING PROGRAM:

```

"BEGIN"
"COMMENT" GREGORY AND KARNEY, CHAPTER 6, EXAMPLE 6,6;
"INTEGER" "PROCEDURE" QRIHRM(A,N,VAL,VR,VI,EM); "CODE" 34371;
"PROCEDURE" INIMAT(LR,UR,LC,UC,A,X); "CODE" 31011;
"PROCEDURE" SCLCOM(AR,AI,N,N1,N2); "CODE" 34360;
"REAL" "ARRAY" A,VR,VI[1:4,1:4],VAL[1:4],EM[0:5]; "INTEGER" I;
INIMAT(1,4,1,4,A,0);
A[1,1]:=A[2,2]:=3;
A[3,2]:=2;A[4,1]:=-2;
A[1,2]:=A[3,3]:=A[3,4]:=A[4,4]:=1;
EM[0]:=EM[2]:=5"-14;EM[4]:=20;
OUTPUT(61,"("("QRIHRM: ")",D/"",QRIHRM(A,4,VAL,VR,VI,EM));
SCLCOM(VR,VI,4,2,3);
OUTPUT(61,"("("EIGENVALUES: ")""");
"FOR" I:=1,2,3,4 "DO" OUTPUT(61,"("/,"("VAL[")",D,"("): ")",
+D,3DB8")",I,VAL[I]);
OUTPUT(61,"("/,"("EIGENVECTORS CORRESPONDING TO")",/,
(" VAL[2] , VAL[3] ")",/)"");
"FOR" I:=1,2,3,4 "DO"
OUTPUT(61,"(+D,+D,"("*I , ")",+D,+D,"("*I")",/)"",
VR[I,2],VI[I,2],VR[I,3],VI[I,3]);
"FOR" I:=1,3,5 "DO"
OUTPUT(61,"("/,"("EM[")",D,"("): ")",+D,DDD"+DD")",I,EM[I])
"END"

```

OUTPUT:

```

QRIHRM: 0
EIGENVALUES:
VAL[1]: +4.828
VAL[2]: +4.000
VAL[3]: =0.000
VAL[4]: =0.828
EIGENVECTORS CORRESPONDING TO
VAL[2] , VAL[3]
+1+0*I , +0=1*I
=1+0*I , +0+1*I
+0=1*I , +1+0*I
+0=1*I , +1+0*I

EM[1]: +6.000"+00
EM[3]: +3.804"=22
EM[5]: +6.000"+00

```

SOURCE TEXT(S) :

```

"CODE" 34368;
"PROCEDURE" EIGVALHRM(A, N, NUMVAL, VAL, EM); "VALUE" N, NUMVAL;
"INTEGER" N, NUMVAL; "ARRAY" A, VAL, EM;
"BEGIN" "ARRAY" D[1:N], BB[1:N - 1];
"PROCEDURE" HSHHRMTRIVAL(A,N,D,BB,EM); "CODE" 34364;
"PROCEDURE" VALSYMTRI(D,BB,N,N1,N2,VAL,EM); "CODE" 34151;
HSHHRMTRIVAL(A, N, D, BB, EM);
VALSYMTRI(D, BB, N, 1, NUMVAL, VAL, EM)
"END" EIGVALHRM;
"EOP"

```

```
"CODE" 34369;
"PROCEDURE" EIGHRM(A, N, NUMVAL, VAL, VECR, VECI, EM);
"VALUE" N, NUMVAL; "INTEGER" N, NUMVAL;
"ARRAY" A, VAL, VECR, VECI, EM;
"BEGIN" "ARRAY" BB, TR, TI[1:N = 1], D, B[1:N];
"PROCEDURE" HSHHRMTRI(A, N, D, B, BB, EM, TR, TI); "CODE" 34363;
"PROCEDURE" VALSYMTRI(D, BB, N, N1, N2, VAL, EM); "CODE" 34151;
"PROCEDURE" VECSYMTRI(D, B, N, N1, N2, VAL, VEC, EM); "CODE" 34152;
"PROCEDURE" BAKHRMTRI(A, N, N1, N2, VECR, VECI, TR, TI); "CODE" 34365;
HSHHRMTRI(A, N, D, B, BB, EM, TR, TI);
VALSYMTRI(D, BB, N, 1, NUMVAL, VAL, EM); B[N] := 0;
VECSYMTRI(D, B, N, 1, NUMVAL, VAL, VECR, EM);
BAKHRMTRI(A, N, 1, NUMVAL, VECR, VECI, TR, TI)
"END" EIGHRM;
"EOP"
```

```
"CODE" 34370;
"INTEGER" "PROCEDURE" QRIVALHRM(A, N, VAL, EM); "VALUE" N;
"INTEGER" N; "ARRAY" A, VAL, EM;
"BEGIN" "ARRAY" B, BB[1:N];
"INTEGER" I;
"PROCEDURE" HSHHRMTRIVAL(A, N, D, BB, EM); "CODE" 34364;
"INTEGER" "PROCEDURE" QRIVALSYMTRI(D, BB, N, EM); "CODE" 34160;
HSHHRMTRIVAL(A, N, VAL, BB, EM); B[N] := BB[N] := 0;
"FOR" I := 1 "STEP" 1 "UNTIL" N := 1 "DO" B[I] := SQRT(BB[I]);
QRIVALHRM := QRIVALSYMTRI(VAL, BB, N, EM)
"END" QRIVALHRM;
"EOP"
```

```
"CODE" 34371;
"INTEGER" "PROCEDURE" QRIHRM(A, N, VAL, VR, VI, EM); "VALUE" N;
"INTEGER" N; "ARRAY" A, VAL, VR, VI, EM;
"BEGIN" "INTEGER" I, J;
"ARRAY" B, BB[1:N], TR, TI[1:N = 1];
"PROCEDURE" HSHHRMTRI(A, N, D, B, BB, EM, TR, TI); "CODE" 34363;
"INTEGER" "PROCEDURE" QRISYMTRI(A, N, D, B, BB, EM); "CODE" 34161;
"PROCEDURE" BAKHRMTRI(A, N, N1, N2, VECR, VECI, TR, TI); "CODE" 34365;
HSHHRMTRI(A, N, VAL, B, BB, EM, TR, TI);
"FOR" I := 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" VR[I, I] := 1;
"FOR" J := I + 1 "STEP" 1 "UNTIL" N "DO" VR[I, J] := VR[J, I] :=
0
"END";
B[N] := BB[N] := 0;
I := QRIHRM := QRISYMTRI(VR, N, VAL, B, BB, EM);
BAKHRMTRI(A, N, I+1, N, VR, VI, TR, TI);
"END" QRIHRM;
"EOP"
```



SECTION 3.3.2.2.1

(JULY 1974)

PAGE 1

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## BRIEF DESCRIPTION :

THIS SECTION CONTAINS THE PROCEDURES VALQRICOM AND QRICOM.  
VALQRICOM CALCULATES THE EIGENVALUES OF A COMPLEX UPPER-HESSSENBERG  
MATRIX WITH A REAL SUBDIAGONAL.  
QRICOM CALCULATES THE EIGENVECTORS AS WELL.

## KEYWORDS :

EIGENVALUES,  
EIGENVECTORS,  
COMPLEX UPPER-HESSSENBERG MATRIX,  
QR-ITERATION.

SUBSECTION: VALQRICOM.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "INTEGER" "PROCEDURE" VALQRICOM(A1, A2, B, N, EM, VAL1, VAL2);  
 "VALUE" N; "INTEGER" N; "ARRAY" A1, A2, B, EM, VAL1, VAL2;

THE MEANING OF THE FORMAL PARAMETERS IS:

A1,A2: <ARRAY IDENTIFIER>;  
 "ARRAY" A1,A2[1:N,1:N];  
 ENTRY:  
 THE REAL PART AND THE IMAGINARY PART OF THE UPPER TRIANGLE OF THE UPPER-HESSENBERG MATRIX MUST BE GIVEN IN THE CORRESPONDING PARTS OF THE ARRAYS A1 AND A2; THE ELEMENTS IN THE UPPER TRIANGLE OF THE ARRAYS A1 AND A2 ARE ALTERED;

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N-1];  
 ENTRY:  
 THE REAL SUBDIAGONAL OF THE UPPER-HESSENBERG MATRIX; THE ELEMENTS OF THE ARRAY B ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY:  
 EM[0]: THE MACHINE PRECISION;  
 EM[1]: AN ESTIMATE OF THE NORM OF THE UPPER-HESSENBERG MATRIX (E.G. THE SUM OF THE INFINITY NORMS OF THE REAL AND IMAGINARY PARTS OF THE MATRIX);  
 EM[2]: THE RELATIVE TOLERANCE FOR THE QR-ITERATION; (E.G. THE MACHINE PRECISION);  
 EM[4]: THE MAXIMUM ALLOWED NUMBER OF ITERATIONS; (E.G. 10 \* N);  
 EXIT:  
 EM[3]: THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL ELEMENTS NEGLECTED;  
 EM[5]: THE NUMBER OF ITERATIONS PERFORMED;  
 EM[5] = EM[4] + 1 IN THE CASE VALQRICOM = 0;

VAL1,VAL2: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL1,VAL2[1:N];  
 EXIT:  
 THE REAL PART AND THE IMAGINARY PART OF THE CALCULATED EIGENVALUES ARE DELIVERED IN THE ARRAYS VAL1 AND VAL2, RESPECTIVELY;

VALQRICOM = 0, PROVIDED THE PROCESS IS COMPLETED WITHIN EM[4] ITERATIONS; OTHERWISE, VALQRICOM = K, THE NUMBER, K, OF EIGENVALUES NOT CALCULATED AND ONLY THE LAST N-K ELEMENTS OF THE ARRAYS VAL1 AND VAL2 ARE APPROXIMATE EIGENVALUES OF THE UPPER-HESSENBERG MATRIX.

PROCEDURES USED:

```

COMKWD      = CP34345,
ROTCOMROW  = CP34358,
ROTCOMCOL  = CP34357,
COMCOLCST  = CP34352,

```

RUNNING TIME: PROPORTIONAL TO  $N^2$  \* NUMBER OF ITERATIONS,

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE QRICOM (THIS SECTION).

EXAMPLE OF USE:

AS A FORMAL TEST OF THE PROCEDURE VALQRICOM THE ZEROS OF THE POLYNOMIAL  $X^4 + (4+2I)X^3 + (5+6I)X^2 + (2+6I)X + 2I$  ARE OBTAINED BY MEANS OF THE CALCULATION OF THE EIGENVALUES OF THE FOLLOWING COMPANION MATRIX:

(SEE WILKINSON AND REINSCH, 1971, CONTRIBUTION II/15)

```

-4-2*I  -5-6*I  -2-6*I   -2*I
  1      0      0      0
  0      1      0      0
  0      0      1      0

```

```

"BEGIN"
"REAL" "ARRAY" A1,A2[1:4,1:4],B[1:3],EM[0:5],VAL1,VAL2[1:4];
"INTEGER" I;
"PROCEDURE" INIMAT(LR,UR,LC,UC,A,X);"CODE" 31011;
"INTEGER" "PROCEDURE" VALQRICOM(A1,A2,B,N,EM,VAL1,VAL2);
"CODE" 34372;
INIMAT(1,4,1,4,A1,0);INIMAT(1,4,1,4,A2,0);
A1[1,1]:=4;A1[1,2]:=5;A1[1,3]:=A2[1,1];A2[1,4]:=2;
A2[1,2]:=A2[1,3];A2[1,3]:=6;
B[1]:=B[2];B[3]:=1;
EM[0]:=5"-14;EM[1]:=27;EM[2]:= "-12;EM[4]:=15;
OUTPUT(61,"("("VALQRICOM: ")",D/"),
      VALQRICOM(A1,A2,B,4,EM,VAL1,VAL2));
OUTPUT(61,"("("EIGENVALUES: ")",/,("REAL PART")",14B,
      ("IMAGINARY PART")",/");
"FOR" I:=1,2,3,4 "DO" OUTPUT(61,"("N,N/"),VAL1[I],VAL2[I]);
OUTPUT(61,"("("EM[3]: ")",D,D"+DD/,("EM[5]: ")",3D)",
      EM[3],EM[5])
"END"

```

OUTPUT:

```

VALQRICOM: 0
EIGENVALUES:
REAL PART          IMAGINARY PART
-1.0000001920467"+000  -1.0000000831019"+000
-9.9999980795324"-001  -9.9999991689805"-001
-1.0000000047492"+000  +1.6824958523393"-007
-9.9999999525076"-001  -1.6824956397352"-007
EM[3]: 3.2"-14
EM[5]: 010

```

SUBSECTION: QRICOM.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "INTEGER" "PROCEDURE" QRICOM(A1,A2,B,N,EM,VAL1,VAL2,VEC1,VEC2);  
 "VALUE" N; "INTEGER" N;  
 "ARRAY" A1, A2, B, EM, VAL1, VAL2, VEC1, VEC2;

THE MEANING OF THE FORMAL PARAMETERS IS:

A1,A2: <ARRAY IDENTIFIER>;  
 "ARRAY" A1,A2[1:N,1:N];  
 ENTRY:  
 THE REAL PART AND THE IMAGINARY PART OF THE UPPER TRIANGLE OF THE UPPER-HESSENBERG MATRIX MUST BE GIVEN IN THE CORRESPONDING PARTS OF THE ARRAYS A1 AND A2;  
 THE ELEMENTS IN THE UPPER TRIANGLE OF THE ARRAYS A1 AND A2 ARE ALTERED;

B: <ARRAY IDENTIFIER>;  
 "ARRAY" B[1:N-1];  
 ENTRY:  
 THE REAL SUBDIAGONAL OF THE UPPER-HESSENBERG MATRIX;  
 THE ELEMENTS OF THE ARRAY B ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY:  
 EM[0]: THE MACHINE PRECISION;  
 EM[1]: AN ESTIMATE OF THE NORM OF THE UPPER-HESSENBERG MATRIX (E.G. THE SUM OF THE INFINITY NORMS OF THE REAL AND IMAGINARY PARTS OF THE MATRIX);  
 EM[2]: THE RELATIVE TOLERANCE FOR THE QR-ITERATION; (E.G. THE MACHINE PRECISION);  
 EM[4]: THE MAXIMUM ALLOWED NUMBER OF ITERATIONS; (E.G. 10 \* N);  
 EXIT:  
 EM[3]: THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL ELEMENTS NEGLECTED;  
 EM[5] THE NUMBER OF ITERATIONS PERFORMED;  
 EM[5]:=EM[4]+1 IN THE CASE QRICOM=0;

VAL1,VAL2: <ARRAY IDENTIFIER>;  
 "ARRAY" VAL1,VAL2[1:N];  
 EXIT:  
 THE REAL PART AND THE IMAGINARY PART OF THE CALCULATED EIGENVALUES ARE DELIVERED IN THE ARRAYS VAL1 AND VAL2, RESPECTIVELY;

VEC1,VEC2: <ARRAY IDENTIFIER>;  
 "ARRAY" VEC1,VEC2[1:N,1:N];  
 EXIT:  
 THE EIGENVECTORS OF THE UPPER-HESSENBERG MATRIX;  
 THE EIGENVECTOR WITH REAL PART VEC1[1:N,J] AND IMAGINARY PART VEC2[1:N,J] CORRESPONDS TO THE EIGENVALUE VAL1[J] + VAL2[J] \* I, J=1,...,N;

QRICOM:=0, PROVIDED THE PROCESS IS COMPLETED WITHIN EM[4]  
 ITERATIONS; OTHERWISE, QRICOM:= THE NUMBER, K, OF EIGENVALUES NOT  
 CALCULATED AND ONLY THE LAST N-K ELEMENTS OF THE ARRAYS VAL1 AND  
 VAL2 ARE APPROXIMATE EIGENVALUES OF THE UPPER-HESSENBERG MATRIX,  
 AND NO USEFUL EIGENVECTORS ARE DELIVERED.

## PROCEDURES USED:

COMKWD = CP34345,  
 ROTCOMROW = CP34358,  
 ROTCOMCOL = CP34357,  
 COMCOLCST = CP34352,  
 COMROWCST = CP34353,  
 MATVEC = CP34011,  
 COMMATVEC = CP34354,  
 COMDIV = CP34342.

REQUIRED CENTRAL MEMORY: TWO AUXILIARY ARRAYS OF ORDER N ARE DECLARED.

RUNNING TIME: PROPORTIONAL TO  $N^2 \times$  NUMBER OF ITERATIONS.

LANGUAGE: ALGOL 60.

THE FOLLOWING HOLDS FOR BOTH PROCEDURES:

## METHOD AND PERFORMANCE:

THE UPPER-HESSENBERG MATRIX IS TRANSFORMED BY MEANS OF FRANCIS' QR  
 ITERATION ( FRANCIS, 1961, AND WILKINSON, 1965 ) INTO A COMPLEX  
 UPPER TRIANGULAR MATRIX. THE EIGENVALUES ARE THE DIAGONAL ELEMENTS  
 OF THE LATTER MATRIX. TO CALCULATE THE EIGENVECTORS WE FIRST SOLVE  
 THE RESULTING TRIANGULAR SYSTEM OF LINEAR EQUATIONS AND  
 SUBSEQUENTLY PERFORM THE CORRESPONDING BACKTRANSFORMATION.

EXAMPLE OF USE:

GRICOM CALCULATES THE EIGENVALUES AND EIGENVECTORS OF THE FOLLOWING MATRIX;

(SEE WILKINSON AND REINSCH, 1971, CONTRIBUTION II/15)

$=4=2*I$	$=5=6*I$	$=2=6*I$	$=2*I$
1	0	0	0
0	1	0	0
0	0	1	0

THE EIGENVECTORS ARE NORMALIZED BY THE PROCEDURE SCLCOM, (SEE SECTION 1.2.11.).

ONLY THE EIGENVECTOR CORRESPONDING TO  $VAL1[I] + VAL2[I] * I$  IS PRINTED BY THE FOLLOWING PROGRAM.

```

"BEGIN"
"REAL" "ARRAY" A1,A2,VEC1,VEC2(1:4,1:4),B(1:3),
           EM(0:5),VAL1,VAL2(1:4);
"INTEGER" I;
"PROCEDURE" SCLCOM(AR,AI,N,N1,N2);"CODE" 34360;
"PROCEDURE" GRICOM(A1,A2,B,N,EM,VAL1,VAL2,VEC1,VEC2);
"CODE" 34373;
"PROCEDURE" INIMAT(LR,UR,LC,UC,A,X);"CODE" 31011;
INIMAT(1,4,1,4,A1,0);INIMAT(1,4,1,4,A2,0);
A1(1,1):=#4;A1(1,2):=#5;A1(1,3):=#A2(1,1);#A2(1,4):=#2;
A2(1,2):=#A2(1,3);#6;
B(1):=#B(2);#B(3);#1;
EM(0):=#5"#14;EM(1):=#27;EM(2):=#"#12;EM(4):=#15;
OUTPUT(61,"("#"GRICOM:")"",D/"")",
        GRICOM(A1,A2,B,4,EM,VAL1,VAL2,VEC1,VEC2));
OUTPUT(61,"("#"EIGENVALUES:")"",/,"("REAL PART)"",14B,
        "("IMAGINARY PART)"",/)"");
"FOR" I:#1,2,3,4 "DO" OUTPUT(61,"("N,N/"")",VAL1(I),VAL2(I));
SCLCOM(VEC1,VEC2,4,1,4);
OUTPUT(61,"("#"FIRST EIGENVECTOR:")"",/,"("REAL PART)"",14B,
        "("IMAGINARY PART)"",/)"");
"FOR" I:#1,2,3,4 "DO" OUTPUT(61,"("N,N/"")",VEC1(I,1),VEC2(I,1));
OUTPUT(61,"("#"EM(3):)"",D,D"+DD/,"("EM(5):)"",3D)"",
        EM(3),EM(5))
"END"

```

OUTPUT:

QRICOM: 0

EIGENVALUES:

REAL PART

=9.9999980795324"-001

=190000001920467"+000

=1.0000000047492"+000

=9.9999999525076"-001

FIRST EIGENVECTOR:

REAL PART

+1.00000000000000"+000

=5.0000004155098"-001

=5.4472417687634"-008

+2.5000014403510"-001

EM[3]: 3.2"-14

EM[5]: 010

IMAGINARY PART

=9.9999991689805"-001

=1.0000000831019"+000

+1.6824958523393"-007

=1.6824956397352"-007

IMAGINARY PART

=1.7763568394003"-015

+5.0000009602339"-001

=5.0000013757436"-001

+2.5000006232645"-001

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## SOURCE TEXT(S) :

```

"CODE" 34372;
"INTEGER" "PROCEDURE" VALGRICOM(A1, A2, B, N, EM, VAL1, VAL2);
"VALUE" N; "INTEGER" N; "ARRAY" A1, A2, B, EM, VAL1, VAL2;
"BEGIN" "INTEGER" M, NM1, I, I1, Q, Q1, MAX, COUNT;
"REAL" R, Z1, Z2, DD1, DD2, CC, G1, G2, K1, K2, HC, A1NN,
A2NN, AIJ1, AIJ2, AI1I, KAPPA, NUI, MUI1, MUI2,
MUIM11, MUIM12, NUIM1, TOL;
"PROCEDURE" COMCOLCST(L,U,J,AR,AI,XR,XI); "CODE" 34352;
"PROCEDURE" ROTCOMCOL(L,U,I,J,AR,AI,CR,CI,S); "CODE" 34357;
"PROCEDURE" ROTCOMROW(L,U,I,J,AR,AI,CR,CI,S); "CODE" 34358;
"PROCEDURE" COMKWD(PR,PI,QR,QI,GR,GI,KR,KI); "CODE" 34345;
TOL:= EM[1] * EM[2]; MAX:= EM[4]; COUNT:= 0; R:= 0;
M:= N; "IF" N > 1 "THEN" HC:= B[N - 1];
IN: NM1:= N - 1;
"FOR" I:= N, I = 1 "WHILE" ("IF" I >= 1 "THEN" ABS(B[I]) > TOL
"ELSE" "FALSE") "DO" Q:= I; "IF" Q > 1 "THEN"
"BEGIN" "IF" ABS(B[Q - 1]) > R "THEN" R:= ABS(B[Q - 1]) "END";
"IF" Q = N "THEN"
"BEGIN" VAL1[N]:= A1[N,N]; VAL2[N]:= A2[N,N]; N:= NM1;
"IF" N > 1 "THEN" HC:= B[N - 1];
"END"
"ELSE"
"BEGIN" DD1:= A1[N,N]; DD2:= A2[N,N]; CC:= B[NM1];
COMKWD((A1[NM1,NM1] = DD1) / 2, (A2[NM1,NM1] = DD2)
/ 2, CC * A1[NM1,N], CC * A2[NM1,N], G1, G2, K1,
K2); "IF" Q = NM1 "THEN"
"BEGIN" VAL1[NM1]:= G1 + DD1; VAL2[NM1]:= G2 + DD2;
VAL1[N]:= K1 + DD1; VAL2[N]:= K2 + DD2;
N:= N - 2; "IF" N > 1 "THEN" HC:= B[N - 1];
"END"
"ELSE"
"BEGIN" COUNT:= COUNT + 1;
"IF" COUNT > MAX "THEN" "GOTO" OUT; Z1:= K1 + DD1;
Z2:= K2 + DD2;
"IF" ABS(CC) > ABS(HC) "THEN" Z1:= Z1 + ABS(CC);
HC:= CC / 2; I:= Q1:= Q + 1;
AIJ1:= A1[Q,Q] = Z1; AIJ2:= A2[Q,Q] = Z2;
AI1I:= B[Q];
KAPPA:= SQRT(AIJ1 ** 2 + AIJ2 ** 2 + AI1I ** 2);
MUI1:= AIJ1 / KAPPA; MUI2:= AIJ2 / KAPPA;
NUI:= AI1I / KAPPA; A1[Q,Q]:= KAPPA;
A2[Q,Q]:= 0; A1[Q1,Q1]:= A1[Q1,Q1] = Z1;
A2[Q1,Q1]:= A2[Q1,Q1] = Z2;
ROTCOMROW(Q1, N, Q, Q1, A1, A2, MUI1, MUI2,
NUI);
ROTCOMCOL(Q, Q, Q, Q1, A1, A2, MUI1, = MUI2, =
NUI); A1[Q,Q]:= A1[Q,Q] + Z1;
A2[Q,Q]:= A2[Q,Q] + Z2; "COMMENT"
    
```



```

"FOR" I1:= Q1 + 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" AIJ1:= A1[I,I]; AIJ2:= A2[I,I];
      AI1I:= B[I];
      KAPPA:= SQRT(AIJ1 ** 2 + AIJ2 ** 2 + AI1I **
      2); MUIM1:= MUI1; MUIM2:= MUI2;
      NUIM1:= NUI; MUI1:= AIJ1 / KAPPA;
      MUI2:= AIJ2 / KAPPA; NUI:= AI1I / KAPPA;
      A1[I1,I1]:= A1[I1,I1] + Z1;
      A2[I1,I1]:= A2[I1,I1] + Z2;
      ROTCOMROW(I1, N, I, I1, A1, A2, MUI1,
      MUI2, NUI); A1[I,I]:= MUIM1 * KAPPA;
      A2[I,I]:= MUIM2 * KAPPA;
      B[I + 1]:= NUIM1 * KAPPA;

      ROTCOMCOL(Q, I, I, I1, A1, A2, MUI1,
      MUI2, NUI); A1[I,I]:= A1[I,I] + Z1;
      A2[I,I]:= A2[I,I] + Z2; I:= I1;
"END";
AIJ1:= A1[N,N]; AIJ2:= A2[N,N];
KAPPA:= SQRT(AIJ1 ** 2 + AIJ2 ** 2);
"IF" ("IF" KAPPA < TOL "THEN" "TRUE" "ELSE" AIJ2 ** 2
<= EM[0] * AIJ1 ** 2) "THEN"
"BEGIN" B[NM1]:= NUI * AIJ1;
      A1[N,N]:= AIJ1 * MUI1 + Z1;
      A2[N,N]:= AIJ1 * MUI2 + Z2
"END"
"ELSE"
"BEGIN" B[NM1]:= NUI * KAPPA; A1NN:= MUI1 * KAPPA;
      A2NN:= MUI2 * KAPPA; MUI1:= AIJ1 / KAPPA;
      MUI2:= AIJ2 / KAPPA;
      COMCOLCST(Q, NM1, N, A1, A2, MUI1, MUI2);
      A1[N,N]:= MUI1 * A1NN + MUI2 * A2NN + Z1;
      A2[N,N]:= MUI1 * A2NN + MUI2 * A1NN + Z2;
"END";
"END"
"END";
"IF" N > 0 "THEN" "GOTO" IN;
OUT: EM[3]:= R; EM[5]:= COUNT; VALGRICOM:= N;
"END" VALGRICOM;
"EOP"

```

"CODE" 34373;

```

"INTEGER" "PROCEDURE" GRICOM(A1, A2, B, N, EM, VAL1, VAL2, VEC1,
VEC2); "VALUE" N; "INTEGER" N;
"ARRAY" A1, A2, B, EM, VAL1, VAL2, VEC1, VEC2;
"BEGIN" "INTEGER" M, NM1, I, I1, J, Q, Q1, MAX, COUNT;
      "REAL" R, Z1, Z2, DD1, DD2, CC, P1, P2, T1, T2, DELTA1,
      DELTA2, MV1, MV2, H, H1, H2, G1, G2, K1, K2, HC,
      AIJ12, AIJ22, A1NN, A2NN, AIJ1, AIJ2, AI1I, KAPPA,
      NUI, MUI1, MUI2, MUIM1, MUIM2, NUIM1, TOL, MACHTOL;
      "ARRAY" TF1, TF2[1:N]; "COMMENT"

```

```

"PROCEDURE" COMKWD(PR,PI,QR,QI,GR,GI,KR,KI); "CODE" 34345;
"PROCEDURE" ROTCOMROW(L,U,I,J,AR,AI,CR,CI,S); "CODE" 34358;
"PROCEDURE" ROTCOMCOL(L,U,I,J,AR,AI,CR,CI,S); "CODE" 34357;
"PROCEDURE" COMCOLCST(L,U,J,AR,AI,XR,XI); "CODE" 34352;
"PROCEDURE" COMROWCST(L,U,I,AR,AI,XR,XI); "CODE" 34353;
"REAL" "PROCEDURE" MATVEC(L,U,I,A,B); "CODE" 34011;
"PROCEDURE" COMMATVEC(L,U,I,AR,AI,BR,BI,RR,RI); "CODE" 34354;
"PROCEDURE" COMDIV(XR,XI,YR,YI,ZR,ZI); "CODE" 34342;
TOL:= EM[1] * EM[2]; MACHTOL:= EM[0] * EM[1];
MAX:= EM[4]; COUNT:= 0; R:= 0; M:= N;
"IF" N > 1 "THEN" HC:= B[N = 1];
"FOR" I:= 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" VEC1[I,I]:= 1; VEC2[I,I]:= 0;
"FOR" J:= I + 1 "STEP" 1 "UNTIL" N "DO" VEC1[I,J]:=
VEC1[J,I]:= VEC2[I,J]:= VEC2[J,I]:= 0
"END";
IN: NM1:= N = 1;
"FOR" I:= N, I = 1 "WHILE" ("IF" I >= 1 "THEN" ABS(B[I]) > TOL
"ELSE" "FALSE") "DO" Q:= I; "IF" Q > 1 "THEN"
"BEGIN" "IF" ABS(B[Q = 1]) > R "THEN" R:= ABS(B[Q = 1]) "END";
"IF" Q = N "THEN"
"BEGIN" VAL1[N]:= A1[N,N]; VAL2[N]:= A2[N,N]; N:= NM1;
"IF" N > 1 "THEN" HC:= B[N = 1];
"END"
"ELSE"
"BEGIN" DD1:= A1[N,N]; DD2:= A2[N,N]; CC:= B[NM1];
P1:= (A1[NM1,NM1] = DD1) * .5;
P2:= (A2[NM1,NM1] = DD2) * .5;
COMKWD(P1, P2, CC * A1[NM1,N], CC * A2[NM1,N], G1,
G2, K1, K2); "IF" Q = NM1 "THEN"
"BEGIN" A1[N,N]:= VAL1[N]:= G1 + DD1;
A2[N,N]:= VAL2[N]:= G2 + DD2;
A1[Q,Q]:= VAL1[Q]:= K1 + DD1;
A2[Q,Q]:= VAL2[Q]:= K2 + DD2;
KAPPA:= SQRT(K1 ** 2 + K2 ** 2 + CC ** 2);
NUI:= CC / KAPPA; MUI1:= K1 / KAPPA;
MUI2:= K2 / KAPPA; AIJ1:= A1[Q,N];
AIJ2:= A2[Q,N]; H1:= MUI1 ** 2 + MUI2 ** 2;
H2:= 2 * MUI1 * MUI2; H:= = NUI * 2;
A1[Q,N]:= H * (P1 * MUI1 + P2 * MUI2) = NUI *
NUI * CC + AIJ1 * H1 + AIJ2 * H2;
A2[Q,N]:= H * (P2 * MUI1 = P1 * MUI2) + AIJ2 *
H1 = AIJ1 * H2;
ROTCOMROW(Q + 2, M, Q, N, A1, A2, MUI1, MUI2,
NUI);
ROTCOMCOL(1, Q = 1, Q, N, A1, A2, MUI1, =
MUI2, = NUI);
ROTCOMCOL(1, M, Q, N, VEC1, VEC2, MUI1, =
MUI2, = NUI); N:= N = 2;
"IF" N > 1 "THEN" HC:= B[N = 1]; B[Q]:= 0
"END"

```

```

"ELSE"
"BEGIN" COUNT:= COUNT + 1;
"IF" COUNT > MAX "THEN" "GOTO" OUT; Z1:= K1 + DD1;
Z2:= K2 + DD2;
"IF" ABS(CC) > ABS(HC) "THEN" Z1:= Z1 + ABS(CC);
HC:= CC / 2; Q1:= Q + 1; AIJ1:= A1(Q,Q) - Z1;
AIJ2:= A2(Q,Q) - Z2; AI1I:= B(Q);
KAPPA:= SQRT(AIJ1 ** 2 + AIJ2 ** 2 + AI1I ** 2);
MUI1:= AIJ1 / KAPPA; MUI2:= AIJ2 / KAPPA;
NUI:= AI1I / KAPPA; A1(Q,Q):= KAPPA;
A2(Q,Q):= 0; A1(Q1,Q1):= A1(Q1,Q1) - Z1;
A2(Q1,Q1):= A2(Q1,Q1) - Z2;
ROTCOMROW(Q1, M, Q, Q1, A1, A2, MUI1, MUI2,
NUI);
ROTCOMCOL(1, Q, Q, Q1, A1, A2, MUI1, - MUI2, -
NUI); A1(Q,Q):= A1(Q,Q) + Z1;
A2(Q,Q):= A2(Q,Q) + Z2;
ROTCOMCOL(1, M, Q, Q1, VEC1, VEC2, MUI1, -
MUI2, - NUI);
"FOR" I:= Q1 "STEP" 1 "UNTIL" NM1 "DO"
"BEGIN" I1:= I + 1; AIJ1:= A1(I,I); AIJ2:= A2(I,I);
AI1I:= B(I);
KAPPA:= SQRT(AIJ1 ** 2 + AIJ2 ** 2 + AI1I **
2); MUIM1:= MUI1; MUIM2:= MUI2;
NUIM1:= NUI; MUI1:= AIJ1 / KAPPA;
MUI2:= AIJ2 / KAPPA; NUI:= AI1I / KAPPA;
A1(I1,I1):= A1(I1,I1) - Z1;
A2(I1,I1):= A2(I1,I1) - Z2;
ROTCOMROW(I1, M, I, I1, A1, A2, MUI1,
MUI2, NUI); A1(I,I):= MUIM1 * KAPPA;
A2(I,I):= - MUIM2 * KAPPA;
B(I - 1):= NUIM1 * KAPPA;
ROTCOMCOL(1, I, I, I1, A1, A2, MUI1, -
MUI2, - NUI); A1(I,I):= A1(I,I) + Z1;
A2(I,I):= A2(I,I) + Z2;
ROTCOMCOL(1, M, I, I1, VEC1, VEC2, MUI1, -
MUI2, - NUI);
"END" "COMMENT"

```

```

AIJ1:= A1(N,N); AIJ2:= A2(N,N); AIJ12:= AIJ1 ** 2;
AIJ22:= AIJ2 ** 2; KAPPA:= SQRT(AIJ12 + AIJ22);
"IF" ("IF" KAPPA < TOL "THEN" "TRUE" "ELSE" AIJ22 <=
EM(0) * AIJ12) "THEN"
"BEGIN" B(NM1):= MUI * AIJ1;
      A1(N,N):= AIJ1 * MUI1 + Z1;
      A2(N,N):= AIJ1 * MUI2 + Z2
"END"
"ELSE"
"BEGIN" B(NM1):= MUI * KAPPA; A1NN:= MUI1 * KAPPA;
      A2NN:= MUI2 * KAPPA; MUI1:= AIJ1 / KAPPA;
      MUI2:= AIJ2 / KAPPA;
      COMCOLCST(1, NM1, N, A1, A2, MUI1, MUI2);
      COMCOLCST(1, NM1, N, VEC1, VEC2, MUI1,
      MUI2);
      COMROWCST(N + 1, M, N, A1, A2, MUI1,
      MUI2);
      COMCOLCST(N, M, N, VEC1, VEC2, MUI1, MUI2);
      A1(N,N):= MUI1 * A1NN + MUI2 * A2NN + Z1;
      A2(N,N):= MUI1 * A2NN + MUI2 * A1NN + Z2;
"END";
"END";
"END";
"IF" N > 0 "THEN" "GOTO" IN;
"FOR" J:= M "STEP" 1 "UNTIL" 2 "DO"
"BEGIN" TF1(J):= 1; TF2(J):= 0; T1:= A1(J,J); T2:= A2(J,J);
"FOR" I:= J - 1 "STEP" 1 "UNTIL" 1 "DO"
"BEGIN" DELTA1:= T1 - A1(I,I); DELTA2:= T2 - A2(I,I);
      COMMATVEC(I + 1, J, I, A1, A2, TF1, TF2, MV1,
      MV2);
      "IF" ABS(DELTA1) < MACHTOL "AND" ABS(DELTA2) <
      MACHTOL "THEN"
      "BEGIN" TF1(I):= MV1 / MACHTOL;
            TF2(I):= MV2 / MACHTOL
      "END"
      "ELSE" COMDIV(MV1, MV2, DELTA1, DELTA2, TF1(I),
      TF2(I));
"END";
"FOR" I:= 1 "STEP" 1 "UNTIL" M "DO" COMMATVEC(1, J, I,
      VEC1, VEC2, TF1, TF2, VEC1(I,J), VEC2(I,J));
"END";
OUT: EM(3):= R; EM(5):= COUNT; GRICOM:= N;
"END" GRICOM;
"EOP"

```

SECTION 3.3.2.2.2

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BRIEF DESCRIPTION :

THIS SECTION CONTAINS THE PROCEDURES EIGVALCOM AND EIGCOM,  
EIGVALCOM CALCULATES THE EIGENVALUES OF A COMPLEX MATRIX AND  
EIGCOM CALCULATES THE EIGENVECTORS AS WELL.

KEYWORDS :

EIGENVALUES,  
EIGENVECTORS,  
COMPLEX MATRICES,  
EQUILIBRATION,  
REDUCTION HESSENBERG FORM,  
HOUSEHOLDER TRANSFORMATION,  
QR-ITERATION.

SUBSECTION: EIGVALCOM.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "INTEGER" "PROCEDURE" EIGVALCOM(AR, AI, N, EM, VALR, VALI);  
 "VALUE" N; "INTEGER" N; "ARRAY" AR, AI, EM, VALR, VALI;

THE MEANING OF THE FORMAL PARAMETERS IS:

AR, AI: <ARRAY IDENTIFIER>;  
 "ARRAY" AR, AI[1:N, 1:N];  
 ENTRY:  
 THE REAL PART AND THE IMAGINARY PART OF THE MATRIX MUST  
 BE GIVEN IN THE ARRAYS AR AND AI, RESPECTIVELY;  
 THE ELEMENTS OF THE ARRAYS AR AND AI ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:7];  
 ENTRY:  
 EM[0]: THE MACHINE PRECISION;  
 EM[2]: THE RELATIVE TOLERANCE FOR THE QR-ITERATION;  
 (E.G. THE MACHINE PRECISION);  
 EM[4]: THE MAXIMUM ALLOWED NUMBER OF QR-ITERATIONS;  
 (E.G. 10 \* N);  
 EM[6]: THE MAXIMUM ALLOWED NUMBER OF ITERATIONS FOR  
 EQUILIBRATING THE ORIGINAL MATRIX (E.G. N\*\*2/2);  
 EXIT;  
 EM[1]: THE EUCLIDEAN NORM OF THE EQUILIBRATED MATRIX;  
 EM[3]: THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
 ELEMENTS NEGLECTED IN THE QR-ITERATION;  
 EM[5]: THE NUMBER OF QR-ITERATIONS PERFORMED;  
 EM[5] := EM[4] + 1 IN THE CASE EIGVALCOM = 0;  
 EM[7]: THE NUMBER OF ITERATIONS PERFORMED FOR  
 EQUILIBRATING THE ORIGINAL MATRIX;

VALR, VALI: <ARRAY IDENTIFIER>;  
 "ARRAY" VALR, VALI[1:N];  
 EXIT;  
 THE REAL PART AND THE IMAGINARY PART OF THE CALCULATED  
 EIGENVALUES ARE DELIVERED IN THE ARRAYS VALR AND VALI,  
 RESPECTIVELY;

EIGVALCOM := 0, PROVIDED THE QR-ITERATION IS COMPLETED WITHIN EM[4]  
 ITERATIONS; OTHERWISE, EIGVALCOM := THE NUMBER, K, OF EIGENVALUES  
 NOT CALCULATED AND ONLY THE LAST N-K ELEMENTS OF THE ARRAYS VALR  
 AND VALI ARE APPROXIMATE EIGENVALUES OF THE ORIGINAL MATRIX.

PROCEDURES USED:

EQILBRCOM = CP34361,  
 COMEUCNRM = CP34359,  
 HSHCOMHES = CP34366,  
 VALQRICOM = CP34372.

REQUIRED CENTRAL MEMORY: FIVE REAL ARRAYS OF ORDER N AND ONE INTEGER ARRAY OF ORDER N ARE DECLARED.

RUNNING TIME: PROPORTIONAL TO  $N \times 2 \times \text{MAX}(N, \text{NUMBER OF ITERATIONS})$ .

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE: SEE EIGCOM (THIS SECTION).

EXAMPLE OF USE: SEE EIGCOM (THIS SECTION).

SUBSECTION: EIGCOM.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:

"INTEGER" "PROCEDURE" EIGCOM(AR, AI, N, EM, VALR, VALI, VR, VI);  
 "VALUE" N; "INTEGER" N; "ARRAY" AR, AI, EM, VALR, VALI, VR, VI;

THE MEANING OF THE FORMAL PARAMETERS IS:

AR, AI: <ARRAY IDENTIFIER>;  
 "ARRAY" AR, AI[1:N, 1:N];  
 ENTRY:  
 THE REAL PART AND THE IMAGINARY PART OF THE MATRIX MUST BE GIVEN IN THE ARRAYS AR AND AI, RESPECTIVELY;  
 THE ELEMENTS OF THE ARRAYS AR AND AI ARE ALTERED;

N: <ARITHMETIC EXPRESSION>;  
 THE ORDER OF THE GIVEN MATRIX;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:7];  
 ENTRY:  
 EM[0]: THE MACHINE PRECISION;  
 EM[2]: THE RELATIVE TOLERANCE FOR THE QR-ITERATION;  
 (E.G. THE MACHINE PRECISION);  
 EM[4]: THE MAXIMUM ALLOWED NUMBER OF QR-ITERATIONS;  
 (E.G.  $10 \times N$ );  
 EM[6]: THE MAXIMUM ALLOWED NUMBER OF ITERATIONS FOR  
 EQUILIBRATING THE ORIGINAL MATRIX (E.G.  $N \times 2/2$ );

EXIT:  
 EM[1]: THE EUCLIDEAN NORM OF THE EQUILIBRATED MATRIX;  
 EM[3]: THE MAXIMUM ABSOLUTE VALUE OF THE SUBDIAGONAL  
 ELEMENTS NEGLECTED IN THE QR-ITERATION;  
 EM[5]: THE NUMBER OF QR-ITERATIONS PERFORMED;  
 EM[5] = EM[4] + 1 IN THE CASE EIGCOM = 0;  
 EM[7]: THE NUMBER OF ITERATIONS PERFORMED FOR  
 EQUILIBRATING THE ORIGINAL MATRIX;

```

VALR,VALI: <ARRAY IDENTIFIER>;
           "ARRAY" VALR,VALI[1:N];
           EXIT;
           THE REAL PART AND THE IMAGINARY PART OF THE CALCULATED
           EIGENVALUES ARE DELIVERED IN THE ARRAYS VALR AND VALI,
           RESPECTIVELY;
VR,VI:    <ARRAY IDENTIFIER>;
           "ARRAY" VR,VI[1:N,1:N];
           EXIT;
           THE EIGENVECTORS OF THE MATRIX;
           THE NORMALIZED EIGENVECTOR WITH REAL PART VR[1:N,J] AND
           IMAGINARY PART VI[1:N,J] CORRESPONDS TO THE EIGENVALUE
           VALR[J] + VALI[J] * I, J=1,...,N;

```

EIGCOM:=0, PROVIDED THE QR-ITERATION IS COMPLETED WITHIN EM[4] ITERATIONS; OTHERWISE, EIGCOM:= THE NUMBER, K, OF EIGENVALUES NOT CALCULATED AND ONLY THE LAST N-K ELEMENTS OF THE ARRAYS VALR AND VALI ARE APPROXIMATE EIGENVALUES OF THE ORIGINAL MATRIX AND NO USEFUL EIGENVECTORS ARE DELIVERED.

PROCEDURES USED:

```

EQILBRCOM = CP34361,
COMEUCNRM = CP34359,
HSHCOMHES = CP34366,
QRICOM    = CP34373,
BAKCOMHES = CP34367,
BAKLBRCOM = CP34362,
SCLCOM    = CP34360,

```

REQUIRED CENTRAL MEMORY: FIVE REAL ARRAYS OF ORDER N AND ONE INTEGER ARRAY OF ORDER N ARE DECLARED.

RUNNING TIME: PROPORTIONAL TO  $N^2 * \text{MAX}(N, \text{NUMBER OF ITERATIONS})$ .

LANGUAGE : ALGOL 60.



THE FOLLOWING HOLDS FOR BOTH PROCEDURES:

METHOD AND PERFORMANCE:

FOR CALCULATING THE EIGENVALUES AND EIGENVECTORS OF A COMPLEX MATRIX WE DISTINGUISH THE FOLLOWING STEPS:

- 1) THE MATRIX IS EQUILIBRATED (SEE ALSO SECTION 3.2.1.1.2.).
- 2) THE EQUILIBRATED MATRIX IS TRANSFORMED INTO HESSENBERG FORM BY MEANS OF HOUSEHOLDER MATRICES (SEE ALSO SECTION 3.2.1.2.2.2.),
- 3) THE HESSENBERG MATRIX IS TRANSFORMED INTO AN UPPER TRIANGULAR MATRIX BY MEANS OF QR-ITERATION WITH SHIFT OF ORIGIN AND DEFLATION (SEE ALSO SECTION 3.3.2.2.1.).

THE DIAGONAL ELEMENTS OF THE UPPER TRIANGULAR MATRIX ARE THE EIGENVALUES OF THE ORIGINAL MATRIX.

THE EIGENVECTORS OF THE ORIGINAL MATRIX ARE OBTAINED BY CALCULATING THE EIGENVECTORS OF THE UPPER TRIANGULAR MATRIX (3) FOLLOWED BY BACKTRANSFORMATIONS CORRESPONDING TO (2) AND (1).

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## EXAMPLE OF USE:

EIGCOM CALCULATES THE EIGENVALUES AND THE EIGENVECTORS OF THE FOLLOWING MATRIX:

(SEE WILKINSON AND REINSCH, 1971, CONTRIBUTION II/15)

```

1+3*I   2+1*I   3+2*I   1+1*I
3+4*I   1+2*I   2+1*I   4+3*I
2+3*I   1+5*I   3+1*I   5+2*I
1+2*I   3+1*I   1+4*I   5+3*I
    
```

ONLY THE EIGENVECTOR CORRESPONDING TO VALR[1] + VALI[1] \* I IS PRINTED BY THE FOLLOWING PROGRAM.

```

"BEGIN"
"INTEGER" "PROCEDURE" EIGCOM(AR,AI,N,EM,VALR,VALI,VR,VI);
"CODE" 34375;
"REAL" "ARRAY" AR,AI,VR,VI[1:4,1:4],EM[0:7],VALR,VALI[1:4];
"INTEGER" I;
AR[1,1]:=AR[1,4]:=AR[2,2]:=AR[3,2]:=AR[4,1]:=AR[4,3]:=
AI[1,2]:=AI[1,4]:=AI[2,3]:=AI[3,3]:=AI[4,2]:=1;
AR[1,2]:=AR[2,3]:=AR[3,1]:=AI[1,3]:=AI[2,2]:=AI[3,4]:=AI[4,1]:=2;
AR[1,3]:=AR[2,1]:=AR[3,3]:=AR[4,2]:=
AI[1,1]:=AI[2,4]:=AI[3,1]:=AI[4,4]:=3;
AR[2,4]:=AI[2,1]:=AI[4,3]:=4;
AR[3,4]:=AR[4,4]:=AI[3,2]:=5;
EM[0]:=5"-14;EM[2]:=5"-12;EM[4]:=10;EM[6]:=10;
OUTPUT(61,"("("EIGCOM: ")",D)"",
        EIGCOM(AR,AI,4,EM,VALR,VALI,VR,VI));
OUTPUT(61,"("/,"("EIGENVALUES:")",/)"");
"FOR" I:=1,2,3,4 "DO" OUTPUT(61,"(2(+D,4D),"(" * I")",/)"",
        VALR[I],VALI[I]);
OUTPUT(61,"("("FIRST EIGENVECTOR:")",/)"");
"FOR" I:=1,2,3,4 "DO" OUTPUT(61,"(2(+D,4D),"(" * I")",/)"",
        VR[I,1],VI[I,1]);
OUTPUT(61,"("("EM[1]: ")",+DD,DD/,"("EM[3]: ")",+D,D"+DD/,
        "EM[5]: ")",+ZD/,"("EM[7]: ")",+ZD)"",EM[1],EM[3],EM[5],EM[7]);
"END"
    
```

## OUTPUT:

```

EIGCOM: 0
EIGENVALUES:
-3,3710-0,7705 * I
+9,7837+9,3225 * I
+1,3657-1,4011 * I
+2,2217+1,8490 * I
FIRST EIGENVECTOR:
-0,5061+0,5835 * I
+1,0000+0,0000 * I
+0,5183-0,7147 * I
-0,5535+0,0188 * I
EM[1]: +15,30
EM[3]: +6,0"-12
EM[5]: +7
EM[7]: +4
    
```

SOURCE TEXT(S) :

```

"CODE" 34374;
  "INTEGER" "PROCEDURE" EIGVALCOM(AR, AI, N, EM, VALR, VALI);
  "VALUE" N; "INTEGER" N; "ARRAY" AR, AI, EM, VALR, VALI;
  "BEGIN" "INTEGER" "ARRAY" INT[1:N];
    "ARRAY" D, B, DEL, TR, TI[1:N];
    "PROCEDURE" HSHCOMHES(AR, AI, N, EM, B, TR, TI, DEL); "CODE" 34366;
    "REAL" "PROCEDURE" COMEUCNRM(AR, AI, LW, N); "CODE" 34359;
    "PROCEDURE" EQILBRCOM(A1, A2, N, EM, D, INT); "CODE" 34361;
    "INTEGER" "PROCEDURE" VALGRICOM(A1, A2, B, N, EM, VAL1, VAL2);
    "CODE" 34372;
    EQILBRCOM(AR, AI, N, EM, D, INT);
    EM[1] := COMEUCNRM(AR, AI, N = 1, N);
    HSHCOMHES(AR, AI, N, EM, B, TR, TI, DEL);
    EIGVALCOM := VALGRICOM(AR, AI, B, N, EM, VALR, VALI)
  "END" EIGVALCOM;
  "EOP"

"CODE" 34375;
  "INTEGER" "PROCEDURE" EIGCOM(AR, AI, N, EM, VALR, VALI, VR, VI);
  "VALUE" N; "INTEGER" N; "ARRAY" AR, AI, EM, VALR, VALI, VR, VI;
  "BEGIN" "INTEGER" I;
    "INTEGER" "ARRAY" INT[1:N];
    "ARRAY" D, B, DEL, TR, TI[1:N];
    "PROCEDURE" EQILBRCOM(A1, A2, N, EM, D, INT); "CODE" 34361;
    "REAL" "PROCEDURE" COMEUCNRM(AR, AI, LW, N); "CODE" 34359;
    "PROCEDURE" HSHCOMHES(AR, AI, N, EM, B, TR, TI, DEL); "CODE" 34366;
    "INTEGER" "PROCEDURE" GRICOM(A1, A2, B, N, EM, VAL1, VAL2, VEC1, VEC2);
    "CODE" 34373;
    "PROCEDURE" BAKCOMHES(AR, AI, TR, TI, DEL, VR, VI, N, N1, N2);
    "CODE" 34367;
    "PROCEDURE" BAKLBRCOM(N, N1, N2, D, INT, VR, VI); "CODE" 34362;
    "PROCEDURE" SCLCOM(AR, AI, N, N1, N2); "CODE" 34360;
    EQILBRCOM(AR, AI, N, EM, D, INT);
    EM[1] := COMEUCNRM(AR, AI, N = 1, N);
    HSHCOMHES(AR, AI, N, EM, B, TR, TI, DEL);
    I := EIGCOM := GRICOM(AR, AI, B, N, EM, VALR, VALI, VR,
    VI); "IF" I = 0 "THEN"
    "BEGIN" BAKCOMHES(AR, AI, TR, TI, DEL, VR, VI, N, 1, N);
      BAKLBRCOM(N, 1, N, D, INT, VR, VI);
      SCLCOM(VR, VI, N, 1, N)
    "END"
  "END" EIGCOM;
  "EOP"

```

SECTION : 3.4.1.2

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PAGE 1

AUTHOR: J.J.G. ADMIRAAL.

INSTITUTE: UNIVERSITY OF AMSTERDAM.

RECEIVED: 751101.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS TWO MAIN AND NINE AUXILIARY PROCEDURES:

THE TWO MAIN PROCEDURES ARE:

- A. QZIVAL FINDS N PAIRS OF SCALARS (ALFA[M], BETA[M]), WHERE BETA[M] IS REAL, SUCH THAT THE MATRIX  $BETA[M] * A - ALFA[M] * B$  IS SINGULAR.
- B. QZI FINDS N PAIRS OF SCALARS (ALFA[M], BETA[M]), WHERE BETA[M] IS REAL, SUCH THAT THE MATRIX  $BETA[M] * A - ALFA[M] * B$  IS SINGULAR; MOREOVER THE GENERALIZED EIGENVECTORS (THE EIGENVECTORS OF THE MATRIX  $BETA[M] * A - ALFA[M] * B$ ) ARE CALCULATED.

THE AUXILIARY PROCEDURES ARE:

- A. HSHDECMUL:  
THIS PROCEDURE CALCULATES REAL MATRICES Q AND R SUCH THAT  $Q.A = R$  WHERE A IS A GIVEN REAL SQUARE MATRIX, Q IS A PRODUCT OF HOUSEHOLDER MATRICES AND R AN UPPERTRIANGULAR MATRIX. MOREOVER Q.B IS FORMED WITH B A GIVEN MATRIX
- B. HESTGL3:  
GIVEN THE REAL SQUARE MATRICES A, B AND X, WITH B AN UPPER TRIANGULAR MATRIX, HESTGL3 CALCULATES THE MATRICES Q, Z, H, R, WHERE Q, Z ARE ORTHOGONAL, H UPPER HESSENBERG AND R AN UPPER TRIANGULAR MATRIX SUCH THAT  $Q.A.Z = H$  AND  $Q.B.Z = R$ . FURTHER:  $A := Q.A.Z$ ;  $B := Q.B.Z$  AND  $X := Q.X.Z$ .
- C. HESTGL2:  
SEE HESTGL3, BUT HERE THE MATRIX X HAS BEEN LEFT OUT.
- D. HSH2COL:  
THIS PROCEDURE CALCULATES A HOUSEHOLDER MATRIX Q SUCH THAT BY PREMULTIPLYING A GIVEN COLUMN VECTOR V BY Q A ZERO ELEMENT IS FORMED IN V. HERE THE VECTOR V IS A COLUMN OF A MATRIX. FURTHER:  $A := Q.A$  AND  $B := Q.B$  WHERE A, B ARE TWO GIVEN REAL MATRICES.

- E. HSH3COL:  
THIS PROCEDURE CALCULATES A HOUSEHOLDER MATRIX Q SUCH THAT BY PREMULTIPLYING A GIVEN COLUMN VECTOR V BY Q TWO SUCCESSIVE ZERO ELEMENTS ARE FORMED IN V. HERE THE VECTOR V IS A COLUMN OF A MATRIX. FURTHER:  $A := Q.A$  AND  $B := Q.B$  WHERE A AND B ARE TWO GIVEN REAL MATRICES.
- F. HSH2ROW3:  
THIS PROCEDURE CALCULATES A HOUSEHOLDER MATRIX Z SUCH THAT BY POSTMULTIPLYING A GIVEN ROWVECTOR V BY Z A ZERO ELEMENT IS FORMED IN V. HERE THE VECTOR V IS A ROW OF A MATRIX. FURTHER:  $A := A.Z$ ;  $B := B.Z$  AND  $X := X.Z$  WHERE A, B, X ARE THREE GIVEN REAL MATRICES.
- G. HSH2ROW2:  
SEE HSH2ROW3, BUT HERE THE MATRIX X HAS BEEN LEFT OUT.
- H. HSH3ROW3:  
THIS PROCEDURE CALCULATES A HOUSEHOLDER MATRIX Z SUCH THAT BY POSTMULTIPLYING A GIVEN ROWVECTOR V BY Z, TWO SUCCESSIVE ZERO ELEMENTS ARE FORMED IN V. HERE THE VECTOR V IS A ROW OF A MATRIX. FURTHER:  $A := A.Z$ ;  $B := B.Z$  AND  $X := X.Z$  WHERE A, B AND X ARE THREE GIVEN REAL MATRICES.
- I. HSH3ROW2:  
SEE HSH3ROW3, BUT HERE THE MATRIX X HAS BEEN LEFT OUT.

KEYWORDS: QZ - ITERATION  
HOUSEHOLDER'S TRANSFORMATION  
GENERALIZED EIGENVALUES  
GENERALIZED EIGENVECTORS  
UPPER HESSENBERG MATRIX  
UPPER TRIANGULAR MATRIX

## REFERENCES:

- [1]. C.B. MOLER AND G.W. STEWART.  
AN ALGORITHM FOR THE GENERALIZED MATRIX EIGENVALUE PROBLEM  $A * X = LAMBDA * B * X$ .  
REPORT STANFORD UNIVERSITY  
STAN-CS-232-71;

SECTION : 3.4.1.2

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SUBSECTION: QZIVAL

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" QZIVAL(N,A,B,ALFR,ALFI,BETA,ITER,EM);  
 "VALUE" N; "INTEGER" N; "ARRAY" A,B,ALFR,ALFI,BETA,EM;  
 "INTEGER" "ARRAY" ITER;  
 "CODE" 34600;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
 THE NUMBER OF ROWS AND COLUMNS OF THE MATRICES A,B

A: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" A[1:N,1:N];  
 ENTRY: THE GIVEN MATRIX;  
 EXIT: A QUASI UPPER-TRIANGULAR MATRIX  
 (SEE METHOD AND PERFORMANCE);

B: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" B[1:N,1:N];  
 ENTRY: THE GIVEN MATRIX;  
 EXIT: AN UPPER-TRIANGULAR MATRIX;

ALFR: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" ALFR[1:N];  
 THE REAL PARTS OF ALFA[1:N]  
 (SEE METHOD AND PERFORMANCE);

ALFI: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" ALFI[1:N];  
 THE IMAGINARY PARTS OF ALFA[1:N];

BETA: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" BETA[1:N];

ITER: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" ITER[1:N];  
 TROUBLE INDICATOR AND ITERATION COUNTER;  
 IF ITER[1]≠0 THEN NO TROUBLE IS SIGNALIZED,  
 FURTHER SEE METHOD AND PERFORMANCE;

EM: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" EM[0:1];  
 ENTRY: EM[0]: THE SMALLEST POSITIVE MACHINE NUMBER;  
 EM[1]: THE RELATIVE PRECISION OF ELEMENTS OF A AND B;

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## PROCEDURES USED:

TAMMAT = CP 34014  
 ELMCOL = CP 34023  
 HSHDECMUL = CP 34602  
 HESTGL2 = CP 34604  
 HSH2COL = CP 34605  
 HSH3COL = CP 34606  
 HSH2ROW2 = CP 34608  
 HSH3ROW2 = CP 34610  
 CHSH2 = CP 34611  
 HSHVECMAT = CP 31070  
 HSHVECTAY = CP 31073

RUNNING TIME: PROPORTIONAL TO  $N \star \star 3$ 

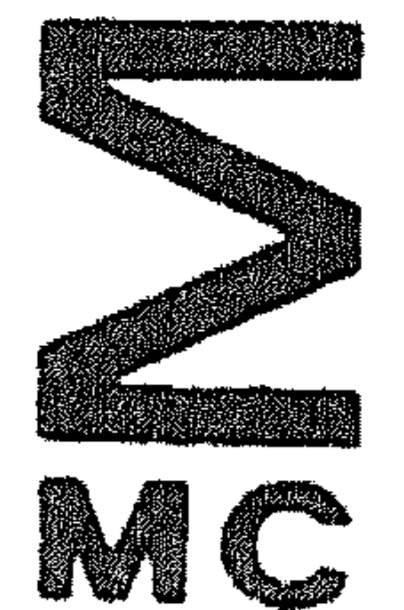
LANGUAGE : ALGOL 60.

## METHOD AND PERFORMANCE:

THE PROCEDURE QZIVAL SOLVES THE GENERALIZED MATRIX EIGENVALUE PROBLEM  $A \star X = \text{LAMBDA} \star B \star X$  BY MEANS OF QZ ITERATION (SEE REF(1)); QZIVAL FINDS  $N$  PAIRS OF SCALARS (ALFA[M], BETA[M]) SUCH THAT  $\text{BETA}[M] \star A - \text{ALFA}[M] \star B$  IS SINGULAR. THE EIGENVALUES OF  $A \star X = \text{LAMBDA} \star B \star X$  CAN BE OBTAINED BY DIVIDING ALFA[M] BY BETA[M], EXCEPT BETA[M] MIGHT BE ZERO. IN THIS ALGORITHM ONLY UNITARY TRANSFORMATIONS ARE APPLIED; A FORTIORI NO INVERSES ARE CALCULATED, SO EITHER A OR B (OR BOTH) MAY BE SINGULAR. BETA[M] IS REAL, ALFA[M] IS COMPLEX. REAL AND IMAGINARY PARTS ARE GIVEN IN ALFR[M] AND ALFI[M]. THE OCCURRENCE OF COMPLEX PAIRS IS ALWAYS IN SUCCESSIVE ELEMENTS, SUCH THAT ALFA[M]/BETA[M] AND ALFA[M+1]/BETA[M+1] ARE COMPLEX CONJUGATE, BUT ALFA[M] AND ALFA[M+1] ARE NOT NECESSARILY CONJUGATE. ONLY REAL ARITHMETIC IS USED IN DE PROCEDURE. IF A AND B WERE REDUCED TO TRIANGULAR FORM BY UNITARY TRANSFORMATIONS, ALFA AND BETA WOULD BE THE DIAGONALS. A AND B ARE ACTUALLY REDUCED TO QUASI-TRIANGULAR FORM HAVING ONLY 1-BY-1 AND 2-BY-2 BLOCKS ON THE DIAGONAL OF A. IF ALFA[M] IS NOT REAL, THEN BETA[M] IS NOT ZERO. ITER IS THE TROUBLE INDICATOR AND ITERATION COUNTER. IF ITER[1]=0 THEN EVERYTHING IS O.K. ITER[M] IS THE NUMBER OF ITERATIONS NEEDED FOR THE M-TH EIGENVALUE. IF ITER[1] THROUGH ITER[M] = -1 THEN THE ITERATION FOR THE M-TH EIGENVALUE DID NOT CONVERGE AND ALFA[1] THROUGH ALFA[M] AND BETA[1] THROUGH BETA[M] ARE PROBABLY INACCURATE.

## EXAMPLE OF USE:

```
"BEGIN" "ARRAY" A,B[1:4,1:4],ALFR,ALFI,BETA[1:4],EM[0:1];
  "INTEGER" "ARRAY" ITER[1:4]; "INTEGER" K,L;
  "PROCEDURE" QZIVAL(N,A,B,ALFR,ALFI,BETA,ITER,EM); "CODE" 34600;
  A[1,1]:=2; A[1,2]:=3; A[1,3]:=-3; A[1,4]:=4;
```



```

A[2,1]:=1; A[2,2]:=-1; A[2,3]:=5; A[2,4]:=1;
A[3,1]:=0; A[3,2]:=2; A[3,3]:=6; A[3,4]:=8;
A[4,1]:=1; A[4,2]:=1; A[4,3]:=0; A[4,4]:=4;
B[1,1]:=1; B[1,2]:=5; B[1,3]:=9; B[1,4]:=0;
B[2,1]:=2; B[2,2]:=6; B[2,3]:=10; B[2,4]:=2;
B[3,1]:=3; B[3,2]:=7; B[3,3]:=11; B[3,4]:=-1;
B[4,1]:=4; B[4,2]:=8; B[4,3]:=12; B[4,4]:=3;
OUTPUT(61, "(" ("(" "A" ), /, 4(4(+ZDBB), /), /)" ", A);
OUTPUT(61, "(" ("(" "B" ), /, 4(4(+ZDBB), /), /)" ", B);
EM[0]:= -294; EM[1]:= -15;
QZIVAL(4, A, B, ALFR, ALFI, BETA, ITER, EM);
"FOR" K:=1 "STEP" 1 "UNTIL" 4 "DO"
OUTPUT(61, "(" ("(" "ITER["), 0, "(" "="), ZD, /)" ", K, ITER[K]);
OUTPUT(61, "(" ("(" "ALFA(REAL PART)" )" 8B, "(" "ALFA(IMAGINARY PART)" )"
3B, "(" "BETA" )" , /)" );
"FOR" K:=1 "STEP" 1 "UNTIL" 4 "DO"
OUTPUT(61, "(" ("3(N), /)" ", ALFR[K], ALFI[K], BETA[K]);
OUTPUT(61, "(" ("/" ("LAMBDA(REAL PART)" )" 6B,
"(" "LAMBDA(IMAGINARY PART)" )" /)" );
"FOR" K:=1 "STEP" 1 "UNTIL" 4 "DO"
"BEGIN" "IF" BETA[K]#0 "THEN"
OUTPUT(61, "(" ("(" "INFINITE" )" 15B, "(" "INDEFINITE" )" /, /)" )
"ELSE" OUTPUT(61, "(" ("2(N), /)" ", ALFR[K]/BETA[K], ALFI[K]/BETA[K])
"END"
"END"

```

A

+2	+3	=3	+4
+1	=1	+5	+1
+0	+2	+6	+8
+1	+1	+0	+1

B

+1	+5	+9	+0
+2	+6	+10	+2
+3	+7	+11	=1
+4	+8	+12	+3

```

ITER[1]= 0
ITER[2]= 0
ITER[3]= 0
ITER[4]= 5

```

ALFA(REAL PART)	ALFA(IMAGINARY PART)	BETA
-4.4347115652167"+000	+0.00000000000000"+000	+0.00000000000000"+000
-5.7288406521003"+000	+0.00000000000000"+000	+2.8441121744896"+000
-8.6671777386054"-001	+2.7607904944916"+000	+8.7617886336960"+000
-4.7262205157527"-001	-1.5054617625576"+000	+4.7778119295757"+000

LAMBDA(REAL PART)	LAMBDA(IMAGINARY PART)
INFINITE	INDEFINITE
-2.0142808372628"+000	+0.00000000000000"+000
-9.8920187429234"-002	+3.1509439566644"-001
-9.8920187429236"-002	-3.1509439566645"-001



## SUBSECTION: QZI

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"PROCEDURE" QZI(N,A,B,X,ALFR,ALFI,BETA,ITER,EM);  
 "VALUE" N; "INTEGER" N; "ARRAY" A,B,X,ALFR,ALFI,BETA,EM;  
 "INTEGER" "ARRAY" ITER;  
 "CODE" 34601;

THE MEANING OF THE FORMAL PARAMETERS IS;

N: <ARITHMETIC EXPRESSION>;  
 THE NUMBER OF ROWS AND COLUMNS OF THE MATRICES A,B AND X;  
 A: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" A(1:N,1:N);  
 ENTRY: THE GIVEN MATRIX A;  
 EXIT: A QUASI UPPER TRIANGULAR MATRIX;  
 (SEE METHOD AND PERFORMANCE);  
 B: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" B(1:N,1:N);  
 ENTRY: THE GIVEN MATRIX B;  
 EXIT: AN UPPER-TRIANGULAR MATRIX;  
 X: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" X(1:N,1:N);  
 ENTRY: THE N\*N UNITY MATRIX;  
 EXIT: THE MATRIX OF EIGENVECTORS,  
 THE EIGENVECTORS ARE STORED IN THE ARRAY X AS FOLLOWS;  
 IF ALFI[M]=0 THEN X[.,M] IS THE M-TH REAL EIGENVECTOR;  
 OTHERWISE, FOR EACH PAIR OF CONSECUTIVE COLUMNS  
 X[.,M] AND X[.,M+1], X[.,M] AND X[.,M+1] ARE THE REAL  
 AND IMAGINARY PARTS OF THE M-TH COMPLEX EIGENVECTOR,  
 X[.,M] AND -X[.,M+1] ARE THE REAL AND IMAGINARY PARTS  
 OF THE M+1 -ST COMPLEX EIGENVECTOR.  
 THE EIGENVECTORS ARE NORMALIZED SUCH THAT THE LARGEST  
 COMPONENT IS 1 OR 1 + 0 \* I.  
 ALFR: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" ALFR(1:N);  
 EXIT: THE REAL PARTS OF ALFA(1:N);  
 ALFI: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" ALFI(1:N);  
 EXIT: THE IMAGINARY PARTS OF ALFA(1:N);  
 BETA: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" BETA(1:N);  
 ITER: <ARRAY IDENTIFIER>;  
 "INTEGER" "ARRAY" ITER(1:N);  
 TROUBLE INDICATOR AND ITERATION COUNTER;  
 IF ITER[1]=0 THEN NO TROUBLE IS SIGNALIZED,  
 FOR FURTHER INFORMATION SEE  
 METHOD AND PERFORMANCE OF PROCEDURE QZIVAL (THIS SECTION).  
 EM: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" EM(0:1);  
 ENTRY: EM[0]: THE SMALLEST POSITIVE MACHINE NUMBER;  
 EM[1]: THE RELATIVE PRECISION OF ELEMENTS OF A AND B;

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## PROCEDURES USED:

```

MATMAT      = CP 34013
TAMMAT      = CP 34014
ELMCOL      = CP 34023
HSHDEC MUL  = CP 34602
HSH2GL3     = CP 34603
HSH2COL     = CP 34605
HSH2ROW3    = CP 34607
HSH3ROW3    = CP 34609
HSH3COL     = CP 34606
CHSH2       = CP 34611
COMDIV      = CP 34342
HSHVECMAT   = CP 31070
HSHVECTAM   = CP 31073

```

RUNNING TIME: PROPORTIONAL TO N \*\* 3;

LANGUAGE : ALGOL 60.

## METHOD AND PERFORMANCE:

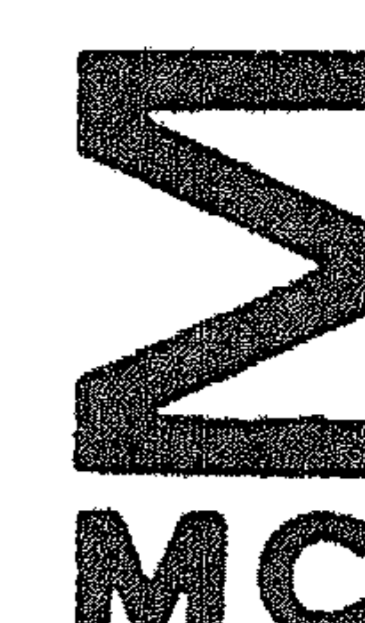
THE PROCEDURE QZI APPLIES THE SAME METHOD AS QZIVAL.

## EXAMPLE OF USE:

```

"BEGIN" "ARRAY" A,B,X[1:4,1:4],ALFR,ALFI,BETA[1:4],EM[0:1];
"INTEGER" "ARRAY" ITER[1:4]; "INTEGER" K,L;
"PROCEDURE" QZI(N,A,B,X,ALFR,ALFI,BETA,ITER,EM); "CODE" 34601;
A[1,1]:=2; A[1,2]:=3; A[1,3]:=3; A[1,4]:=4;
A[2,1]:=1; A[2,2]:=1; A[2,3]:=5; A[2,4]:=1;
A[3,1]:=0; A[3,2]:=2; A[3,3]:=6; A[3,4]:=8;
A[4,1]:=1; A[4,2]:=1; A[4,3]:=0; A[4,4]:=4;
B[1,1]:=1; B[1,2]:=5; B[1,3]:=9; B[1,4]:=0;
B[2,1]:=2; B[2,2]:=6; B[2,3]:=10; B[2,4]:=2;
B[3,1]:=3; B[3,2]:=7; B[3,3]:=11; B[3,4]:=1;
B[4,1]:=4; B[4,2]:=8; B[4,3]:=12; B[4,4]:=3;
"FOR" K:=1,2,3,4 "DO" "FOR" L:=1,2,3,4 "DO"
X[K,L]:="IF" K=L "THEN" 1 "ELSE" 0;
OUTPUT(61,"("("A"),/,4(4(+ZDBB),/),/)"",A);
OUTPUT(61,"("("B"),/,4(4(+ZDBB),/),/)"",B);
EM[0]:="=294;EM[1]:="=15;
QZI(4,A,B,X,ALFR,ALFI,BETA,ITER,EM);

```



```

"FOR" K:=1 "STEP" 1 "UNTIL" 4 "DO"
OUTPUT(61, "("("ITER["), D, "("(")=", ZD, "/"")", K, ITER[K]);
OUTPUT(61, "("("/("EIGENVECTORS")", /, 4(4(+D.8D"+2D2B), /), /")", X);
OUTPUT(61, "("("ALFA(REAL PART)")"8B, "("ALFA(IMAGINARY PART)")"
9B, "("BETA")", /")");
"FOR" K:=1 "STEP" 1 "UNTIL" 4 "DO"
OUTPUT(61, "("3(N), /")", ALFR[K], ALFI[K], BETA[K]);
OUTPUT(61, "("("/("LAMBDA(REAL PART)")"6B,
"("LAMBDA(IMAGINARY PART)")"/")");
"FOR" K:=1 "STEP" 1 "UNTIL" 4 "DO"
"BEGIN" "IF" BETA[K]=0 "THEN"
    OUTPUT(61, "("("INFINITE")"15B, "("INDEFINITE")"/")"
"ELSE"
    OUTPUT(61, "("2(N), /")", ALFR[K]/BETA[K], ALFI[K]/BETA[K])
"END"
"END"

```

A

+2	+3	=3	+4
+1	=1	+5	+1
+0	+2	+6	+8
+1	+1	+0	+4

B

+1	+5	+9	+0
+2	+6	+10	+2
+3	+7	+11	=1
+4	+8	+12	+3

```

ITER[1]= 0
ITER[2]= 0
ITER[3]= 0
ITER[4]= 5

```

EIGENVECTORS

=5.00000000"=01	+1.00000000"+00	=6.29204867"=01	+6.52026261"=01
+1.00000000"+00	=3.82541766"=02	+1.00000000"+00	+0.00000000"+00
=5.00000000"=01	=3.04677732"=02	+1.65896051"=01	+1.09306265"=01
=4.35116786"=15	=7.63328122"=01	=5.84845537"=01	+1.77430910"=01

ALFA(REAL PART)

=4.4347115652167"+000
=5.7288406521003"+000
=8.6671777386054"=001
=4.7262205157527"=001

ALFA(IMAGINARY PART)

+0.00000000000000"+000
+0.00000000000000"+000
+2.7607904944916"+000
=1.5054617625576"+000

BETA

+0.00000000000000"+000
+2.8441121744896"+000
+8.7617886336960"+000
+4.7778119295757"+000

LAMBDA(REAL PART)

INFINITE
=2.0142908372628"+000
=9.8920187429234"=002
=9.8920187429236"=002

LAMBDA(IMAGINARY PART)

INDEFINITE
+0.00000000000000"+000
+3.1509439566644"=001
=3.1509439566645"=001

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SUBSECTION: HSHDECMUL.

CALLING SEQUENCE:

THE HEADING OF THIS PROCEDURE IS:  
"PROCEDURE" HSHDECMUL(N,A,B,DWARF);  
"VALUE" N,DWARF; "INTEGER" N; "REAL" DWARF; "ARRAY" A,B;  
"CODE" 34602;

THE MEANING OF THE FORMAL PARAMETERS IS:  
N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE GIVEN MATRICES;  
A: <ARRAY IDENTIFIER>;  
"REAL" "ARRAY" A[1:N,1:N];  
ENTRY: THE GIVEN MATRIX A;  
EXIT: THE TRANSFORMED MATRIX Q.A (SEE BRIEF DESCRIPTION);  
B: <ARRAY IDENTIFIER>;  
"REAL" "ARRAY" B[1:N,1:N];  
ENTRY: THE GIVEN MATRIX B;  
EXIT: THE UPPER TRIANGULAR MATRIX Q.B (SEE BRIEF DESCRIPTION);  
DWARF: < ARITHMETIC EXPRESSION>;  
THE SMALLEST POSITIVE MACHINE NUMBER.

PROCEDURES USED:

TAMMAT = CP 34014;  
HSHVECMAT = CP 31070.

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

FOR EACH MATRIX COLUMN A[I] A HOUSEHOLDER MATRIX Q IS FORMED,  
SUCH THAT Q.A[I] HAS ONLY ZERO ELEMENTS BELOW THE DIAGONAL ELEMENT.  
WHEN SUCCESSIVELY FOR I = 1,2,...,N-1 THESE TRANSFORMATIONS HAVE  
BEEN PERFORMED, THE MATRIX A HAS BEEN CHANGED IN AN UPPER TRIANGULAR  
MATRIX.

THE SAME TRANSFORMATIONS ARE PERFORMED ON THE MATRIX B

EXAMPLE OF USE:

THE PROCEDURE HSHDECMUL IS USED IN QZI AND QZIVAL (THIS SECTION).

SUBSECTION: HESTGL3:

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
"PROCEDURE" HESTGL3(N,A,B,X);  
"VALUE" N; "INTEGER" N; "ARRAY" A,B,X;  
"CODE" 34603;

THE MEANING OF THE FORMAL PARAMETERS IS:  
N: <ARITHMETIC EXPRESSION>;  
THE ORDER OF THE GIVEN MATRICES;  
A: <ARRAY IDENTIFIER>;  
"REAL" "ARRAY" A[1:N,1:N];  
ENTRY: THE GIVEN MATRIX A;  
EXIT: THE UPPER HESSENBERG MATRIX Q.A.Z (SEE BRIEF DESCRIPTION);  
B: <ARRAY IDENTIFIER>;  
"REAL" "ARRAY" B[1:N,1:N];  
ENTRY: THE GIVEN UPPER TRIANGULAR MATRIX B;  
EXIT: THE UPPER TRIANGULAR MATRIX Q.B.Z (SEE BRIEF DESCRIPTION);  
X: <ARRAY IDENTIFIER>;  
"REAL" "ARRAY" X[1:N,1:N];  
ENTRY: THE GIVEN MATRIX X;  
EXIT: THE TRANSFORMED MATRIX Q.X.Z (SEE BRIEF DESCRIPTION);

PROCEDURES USED:  
HSH2COL = CP 34605  
HSH2ROW3 = CP 34607

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:  
THE REDUCTION OF THE MATRIX A TO UPPER HESSENBERG FORM  
WHILE PRESERVING THE TRIANGULARITY OF THE MATRIX B  
IS THE RESULT OF A NUMBER OF STEPS, WHICH DO THE FOLLOWING  
ACTIONS: INTRODUCING A ZERO ELEMENT IN A AND RESTORING  
THE DISTURBED ZERO IN B, WITHOUT DISTURBING THE ZERO  
INTRODUCED IN A. THIS IS DONE BY PRE-AND POSTMULTIPLICATIONS OF  
HOUSEHOLDER MATRICES.  
THE MATRIX X SHARES THE TRANSFORMATION.  
FOR FURTHER DETAILS SEE [1]

EXAMPLE OF USE:

THE PROCEDURE HESTGL3 IS USED IN QZI (THIS SECTION).

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SUBSECTION: HESTGL2:

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
"PROCEDURE" HESTGL2(N,A,B); "VALUE" N; "INTEGER" N; "ARRAY" A,B;  
"CODE" 34604;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;

THE ORDER OF THE GIVEN MATRICES;

A: <ARRAY IDENTIFIER>;

"REAL" "ARRAY" A[1:N,1:N];

ENTRY: THE GIVEN MATRIX A;

EXIT: THE UPPER HESSENBERG MATRIX Q.A.Z (SEE BRIEF DESCRIPTION);

B: <ARRAY IDENTIFIER>;

"REAL" "ARRAY" B[1:N,1:N];

ENTRY: THE GIVEN UPPER TRIANGULAR MATRIX B

EXIT: THE UPPER TRIANGULAR MATRIX Q.B.Z (SEE BRIEF DESCRIPTION);

PROCEDURES USED:

HSH2COL = CP 34605

HSH2R042 = CP 34608

LANGUAGE: ALGOL 60.

METHODE AND PERFORMANCE:

SEE HESTGL3, BUT HERE THE MATRIX X HAS BEEN LEFT OUT.

EXAMPLE OF USE:

THE PROCEDURE HESTGL2 IS USED IN QZIVAL (THIS SECTION).

SECTION : 3.4.1.2

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SUBSECTION HSH2COL:

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" HSH2COL(LA, LB, U, I, A1, A2, A, B); "VALUE" LA, LB, U, I, A1, A2;  
 "INTEGER" LA, LB, U, I; "REAL" A1, A2; "ARRAY" A, B;  
 "CODE" 34605;

THE MEANING OF THE FORMAL PARAMETERS IS:  
 LA: <ARITHMETIC EXPRESSION>;  
 THE LOWER BOUND OF THE RUNNING COLUMN SUBSCRIPT OF A;  
 LB: <ARITHMETIC EXPRESSION>;  
 THE LOWER BOUND OF THE RUNNING COLUMN SUBSCRIPT OF B;  
 U: <ARITHMETIC EXPRESSION>;  
 THE UPPER BOUND OF THE RUNNING COLUMN SUBSCRIPTS  
 OF A AND B.  
 I: <ARITHMETIC EXPRESSION>;  
 THE LOWERBOUND OF THE RUNNING ROW SUBSCRIPTS OF A AND B.  
 I+1 IS THE UPPERBOUND.  
 A1: <ARITHMETIC EXPRESSION>;  
 THE I-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED.  
 A2: <ARITHMETIC EXPRESSION>;  
 THE (I+1)-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;  
 A: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" A[I:I+1, LA:U];  
 ENTRY THE GIVEN MATRIX A;  
 EXIT: THE TRANSFORMED MATRIX Q.A (SEE BRIEF DESCRIPTION);  
 B: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" B[I:I+1, LB:U];  
 ENTRY: THE GIVEN MATRIX B;  
 EXIT: THE TRANSFORMED MATRIX Q.B (SEE BRIEF DESCRIPTION);

PROCEDURES USED:

HSHVECMAT = CP 31070

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

WHEN THE CALCULATED HOUSEHOLDERMATRIX Q PREMULTIPLIES  
 A MATRIX M, ONLY ROWS I AND I+1 ARE CHANGED.  
 IF THE ELEMENTS I AND I+1 IN A COLUMN OF M ARE ZERO, THEY  
 REMAIN ZERO IN Q.M.  
 THEREFORE ONLY THE SUBMATRICES A[I:I+1, LA:U] AND  
 B[I:I+1, LB:U] ARE CHANGED, WHERE Q.A AND Q.B ARE  
 OVERWRITTEN IN A RESP B.

EXAMPLE OF USE: THE PROCEDURE HSH2COL IS USED IN QZI AND QZIVAL,  
 (THIS SECTION).

SECTION : 3.4.1.2

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SUBSECTION HSH3COL:

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

"PROCEDURE" HSH3COL(LA, LB, U, I, A1, A2, A3, A, B);

"VALUE" LA, LB, U, I, A1, A2, A3; "INTEGER" LA, LB, I, U; "REAL" A1, A2, A3;

"ARRAY" A, B;

"CODE" 34606;

THE MEANING OF THE FORMAL PARAMETER IS:

LA: &lt;ARITHMETIC EXPRESSION&gt;;

THE LOWERBOUND OF THE RUNNING COLUMN SUBSCRIPT OF A;

LB: &lt;ARITHMETIC EXPRESSION&gt;;

THE LOWERBOUND OF THE RUNNING COLUMN SUBSCRIPT OF B;

U: &lt;ARITHMETIC EXPRESSION&gt;;

THE UPPERBOUND OF THE RUNNING COLUMN SUBSCRIPT OF A AND B;

I: &lt;ARITHMETIC EXPRESSION&gt;;

THE LOWERBOUND OF THE RUNNING ROW SUBSCRIPT OF A AND B,  
I+2 IS THE UPPERBOUND;

A1: &lt;ARITHMETIC EXPRESSION&gt;;

THE I-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;

A2: &lt;ARITHMETIC EXPRESSION&gt;;

THE (I+1)-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;

A3: &lt;ARITHMETIC EXPRESSION&gt;;

THE (I+2)-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED.

A: &lt;ARRAY IDENTIFIER&gt;;

"REAL" "ARRAY" A[I:I+2, LA:U];

ENTRY: THE GIVEN MATRIX A;

EXIT: THE TRANSFORMED MATRIX Q.A (SEE BRIEF DESCRIPTION);

B: &lt;ARRAY IDENTIFIER&gt;;

"REAL" "ARRAY" B[I:I+2, LB:U];

ENTRY: THE GIVEN MATRIX B;

EXIT: THE TRANSFORMED MATRIX Q.B (SEE BRIEF DESCRIPTION);

PROCEDURES USED: HSHVECMAT = CP 31070;

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

WHEN THE CALCULATED HOUSEHOLDER MATRIX Q PREMULTIPLIES A MATRIX  
H, ONLY ROWS I, (I+1) AND (I+2) ARE CHANGED.IF THE ELEMENTS I, I+1 AND I+2 ARE ZERO, THEN THEY REMAIN ZERO  
IN Q.A.THEREFORE ONLY THE SUBMATRICES A[I:I+2, LA:U] AND B[I:I+2, LB:U]  
ARE CHANGED, WHERE Q.A AND Q.B ARE OVERWRITTEN IN A RESP B.EXAMPLE OF USE: THE PROCEDURE HSH3COL IS USED IN QZI AND QZIVAL  
(THIS SECTION).



SECTION : 3.4.1.2

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SUBSECTION HSH2ROW3:

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" HSH2ROW3(L,UA,UB,UX,J,A1,A2,A,B,X);  
 "VALUE" L,UA,UB,UX,J,A1,A2; "INTEGER" L,UA,UB,UX,J;  
 "REAL" A1,A2; "ARRAY" A,B,X;  
 "CODE" 34607;

THE MEANING OF THE FORMAL PARAMETERS IS:

L: <ARITHMETIC EXPRESSION>;  
 THE LOWERBOUND OF THE RUNNING ROW SUBSCRIPT OF A,B AND X;  
 UA: <ARITHMETIC EXPRESSION>;  
 THE UPPERBOUND OF THE RUNNING ROW SUBSCRIPT OF A;  
 UB: <ARITHMETIC EXPRESSION>;  
 THE UPPERBOUND OF THE RUNNING ROW SUBSCRIPT OF B;  
 UX: <ARITHMETIC EXPRESSION>;  
 THE UPPERBOUND OF THE RUNNING ROW SUBSCRIPT OF X;  
 J: <ARITHMETIC EXPRESSION>;  
 THE LOWERBOUND OF THE RUNNING COLUMN SUBSCRIPT OF A,B AND X;  
 J+1 IS THE UPPERBOUND;  
 A1: <ARITHMETIC EXPRESSION>;  
 THE J-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;  
 A2: <ARITHMETIC EXPRESSION>;  
 THE (J+1)-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;  
 A: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" A(L:UA,J:J+1);  
 ENTRY: THE GIVEN MATRIX A;  
 EXIT: THE TRANSFORMED MATRIX A.Z (SEE BRIEF DESCRIPTION);  
 B: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" B(L:UB,J:J+1);  
 ENTRY: THE GIVEN MATRIX B;  
 EXIT: THE TRANSFORMED MATRIX B.Z (SEE BRIEF DESCRIPTION);  
 X: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" X(L:UX,J:J+1);  
 ENTRY: THE GIVEN MATRIX X;  
 EXIT: THE TRANSFORMED MATRIX X.Z (SEE BRIEF DESCRIPTION);

PROCEDURES USED: HSHVECTAM = CP 31073;

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

WHEN THE CALCULATED HOUSEHOLDERMATRIX Z POSTMULTIPLIES  
 A MATRIX M, ONLY COLUMNS J AND J+1 ARE CHANGED.  
 IF THE ELEMENTS J AND J+1 IN A ROW OF M ARE ZERO, THEN  
 THEY REMAIN ZERO IN M.Z  
 THEREFORE ONLY THE SUBMATRICES A(L:UA,J:J+1),B(L:UB,J:J+1)  
 AND X(L:UX,J:J+1) ARE CHANGED, WHERE A.Z, B.Z AND X.Z ARE  
 OVERWRITTEN IN RESP. A,B AND X.

EXAMPLE OF USE: THE PROCEDURE HSH2ROW3 IS USED IN QZI (THIS SECTION).

SECTION : 3.4.1.2

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SUBSECTION HSH2ROW2:

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE HSH2ROW2(LA, LB, UA, UB, J, A1, A2, A, B); "VALUE" LA, LB, UA,  
 UB, J, A1, A2; "INTEGER" LA, LB, UA, UB, J; "REAL" A1, A2; "ARRAY" A, B;  
 "CODE" 34608;

THE MEANING OF THE FORMAL PARAMETERS IS:

LA: <ARITHMETIC EXPRESSION>;  
 THE LOWERBOUND OF THE RUNNING ROW SUBSCRIPT OF A;

LB: <ARITHMETIC EXPRESSION>;  
 THE LOWERBOUND OF THE RUNNING ROW SUBSCRIPT OF B;

UA: <ARITHMETIC EXPRESSION>;  
 THE UPPERBOUND OF THE RUNNING ROW SUBSCRIPT OF A;

UB: <ARITHMETIC EXPRESSION>;  
 THE UPPERBOUND OF THE RUNNING ROW SUBSCRIPT OF B;

J: <ARITHMETIC EXPRESSION>;  
 THE LOWERBOUND OF THE RUNNING COLUMN SUBSCRIPT OF A AND B;  
 J+1 IS THE UPPERBOUND;

A1: <ARITHMETIC EXPRESSION>;  
 THE J-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;

A2: <ARITHMETIC EXPRESSION>;  
 THE (J+1)-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;

A: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" A(LA;UA, J;J+1);  
 ENTRY: THE GIVEN MATRIX A;  
 EXIT: THE TRANSFORMED MATRIX A.Z (SEE BRIEF DESCRIPTION);

B: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" B(LB;UB, J;J+1);  
 ENTRY: THE GIVEN MATRIX B;  
 EXIT: THE TRANSFORMED MATRIX B.Z (SEE BRIEF DESCRIPTION);

PROCEDURES USED: HSHVECTAN = CP 31073;

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SEE HSH2ROW3, BUT HERE THE MATRIX X HAS BEEN LEFT OUT.

EXAMPLE OF USE:

THE PROCEDURE HSH2ROW2 IS USED IN QZIVAL,  
 (THIS SECTION).

SECTION : 3.4.1.2

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SUBSECTION: HSH3ROW3.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:

```
"PROCEDURE" HSH3ROW3(L,U,UX,J,A1,A2,A3,A,B,X);
"VALUE" L,U,UX,J,A1,A2,A3; "INTEGER" L,U,UX,J; "REAL" A1,A2,A3;
"ARRAY" A,B,X;
"CODE" 34609;
```

THE MEANING OF THE FORMAL PARAMETERS IS:

```
L: <ARITHMETIC EXPRESSION>;
   THE LOWERBOUND OF THE RUNNING ROW SUBSCRIPT OF A AND B AND X;
U: <ARITHMETIC EXPRESSION>;
   THE UPPERBOUND OF THE RUNNING ROW SUBSCRIPT OF A AND B;
UX: <ARITHMETIC EXPRESSION>;
   THE UPPERBOUND OF THE RUNNING ROW SUBSCRIPT OF X;
J: <ARITHMETIC EXPRESSION>;
   THE LOWERBOUND OF THE RUNNING COLUMN SUBSCRIPT OF A,B AND X;
   J+2 IS THE UPPERBOUND;
A1: <ARITHMETIC EXPRESSION>;
   THE J-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;
A2: <ARITHMETIC EXPRESSION>;
   THE (J+1)-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;
A3: <ARITHMETIC EXPRESSION>;
   THE (J+2)-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;
A: <ARRAY IDENTIFIER>;
   "REAL" "ARRAY" A[L:U,J:J+2];
   ENTRY: THE GIVEN MATRIX A;
   EXIT: THE TRANSFORMED MATRIX A.Z (SEE BRIEF DESCRIPTION);
B: <ARRAY IDENTIFIER>;
   "REAL" "ARRAY" B[L:U,J:J+2];
   ENTRY: THE GIVEN MATRIX B;
   EXIT: THE TRANSFORMED MATRIX B.Z (SEE BRIEF DESCRIPTION);
X: <ARRAY IDENTIFIER>;
   "REAL" "ARRAY" X[L:UX,J:J+2];
   ENTRY: THE GIVEN MATRIX X;
   EXIT: THE TRANSFORMED MATRIX X.Z (SEE BRIEF DESCRIPTION);
```

PROCEDURES USED: HSHVECTAM \* CP 31073;

LANGUAGE: ALGOL 60;

METHOD AND PERFORMANCE:

WHEN THE CALCULATED HOUSEHOLDERMATRIX Z POSTMULTIPLIES A MATRIX M, ONLY COLUMNS J, J+1 AND J+2 ARE CHANGED. IF THE ELEMENTS J, J+1 AND J+2 IN A ROW OF M ARE ZERO, THEN THEY REMAIN ZERO IN M.Z. THEREFORE ONLY THE SUBMATRICES A[L:U,J:J+2], B[L:U,J:J+2] AND X[L:UX,J:J+2] ARE CHANGED, WHERE A.Z, B.Z AND X.Z ARE OVERWRITTEN ON RESP. A, B AND X;

EXAMPLE OF USE: THE PROCEDURE HSH3ROW3 IS USED IN QZI (THIS SECTION).

SECTION : 3.4.1.2

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SUBSECTION: HSH3ROW2.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE IS:  
 "PROCEDURE" HSH3ROW2(LA, LB, U, J, A1, A2, A3, A, B);  
 "VALUE" LA, LB, U, J, A1, A2, A3; "INTEGER" LA, LB, U, J;  
 "REAL" A1, A2, A3; "ARRAY" A, B;  
 "CODE" 34610;

THE MEANING OF THE FORMAL PARAMETERS IS:  
 LA: <ARITHMETIC EXPRESSION>;  
 THE LOWERBOUND OF THE RUNNING ROW SUBSCRIPT OF A;  
 LB: <ARITHMETIC EXPRESSION>;  
 THE LOWERBOUND OF THE RUNNING ROW SUBSCRIPT OF B;  
 U: <ARITHMETIC EXPRESSION>;  
 THE UPPERBOUND OF THE RUNNING ROW SUBSCRIPT OF A AND B;  
 J: <ARITHMETIC EXPRESSION>;  
 THE LOWERBOUND OF THE RUNNING COLUMN SUBSCRIPT OF A AND B,  
 J+2 IS THE UPPERBOUND;  
 A1: <ARITHMETIC EXPRESSION>;  
 THE J-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;  
 A2: <ARITHMETIC EXPRESSION>;  
 THE (J+1)-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;  
 A3: <ARITHMETIC EXPRESSION>;  
 THE (J+2)-TH COMPONENT OF THE VECTOR TO BE TRANSFORMED;  
 A: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" A(LA:U, J:J+2);  
 ENTRY: THE GIVEN MATRIX A;  
 EXIT: THE TRANSFORMED MATRIX A.Z (SEE BRIEF DESCRIPTION);  
 B: <ARRAY IDENTIFIER>;  
 "REAL" "ARRAY" B(LB:U, J:J+2);  
 ENTRY: THE GIVEN MATRIX B;  
 EXIT: THE TRANSFORMED MATRIX B.Z (SEE BRIEF DESCRIPTION);

PROCEDURES USED: HSHVECTAM # CP 31073;

LANGUAGE: ALGOL 60.

METHOD AND PERFORMANCE:

SEE HSH3ROW3, BUT HERE THE MATRIX X HAS BEEN LEFT OUT.

EXAMPLE OF USE: HSH3ROW2 IS USED IN QZIVAL (THIS SECTION).

## SOURCE TEXTS:

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"CODE" 34600;
"PROCEDURE" QZIVAL(N,A,B,ALFR,ALFI,BETA,ITER,EM);
"VALUE" N;"INTEGER" N;"ARRAY" A,B,ALFR,ALFI,BETA,EM;
"INTEGER" "ARRAY" ITER;
"BEGIN" "REAL" DWARF,EPS,EPSA,EPSB;
"PROCEDURE" ELMCOL(L,U,I,J,A,B,X);"CODE" 34023;
"PROCEDURE" HSHDECMUL(N,A,B,DWARF);"CODE" 34602;
"PROCEDURE" HESTGL2(N,A,B);"CODE" 34604;
"PROCEDURE" HSH2ROW2(LA,LB,UA,UB,J,A1,A2,A,B);"CODE" 34608;
"PROCEDURE" HSH3ROW2(LA,LB,U,J,A1,A2,A3,A,B);"CODE" 34610;
"PROCEDURE" HSH2COL(LA,LB,U,I,A1,A2,A,B);"CODE" 34605;
"PROCEDURE" HSH3COL(LA,LB,U,I,A1,A2,A3,A,B);"CODE" 34606;
"PROCEDURE" CHSH2(A1R,A1I,A2R,A2I,C,SR,SI);"CODE" 34611;
"PROCEDURE" HSHVECMAT(LR,UR,LC,UC,X,U,A);"CODE" 31070;
"PROCEDURE" HSHVECTAM(LR,UR,LC,UC,X,U,A);"CODE" 31073;
"PROCEDURE" QZIT(N,A,B,EPS,EPSA,EPSB,ITER);"VALUE" N,EPS;
"REAL" EPS,EPSA,EPSB;"INTEGER" N;"INTEGER" "ARRAY" ITER;"ARRAY" A,B;
"BEGIN" "REAL" ANORM,BNORM,ANI,BNI,CONST,A10,A20,A30,B11,
      B22,B33,B44,A11,A12,A21,A22,A33,A34,A43,A44,B12,B34,OLD1,OLD2;
"INTEGER" I,Q,M,M1,Q1,J,K,K1,K2,K3,KM1;"BOOLEAN" STATIONARY;
ANORM:=BNORM:=0;"FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" BNI:=0;ITER[I]:=0;ANI:=0;"IF" I>1"THEN"ABS(A[I,I-1])"ELSE" 0;
      "FOR" J:=I "STEP" 1 "UNTIL" N "DO"
      "BEGIN" ANI:=ANI+ABS(A[I,J]);BNI:=BNI+ABS(B[I,J])
      "END";"IF" ANI>ANORM "THEN" ANORM:=ANI;"IF" BNI>BNORM"THEN"
      BNORM:=BNI
"END";"IF" ANORM=0 "THEN" ANORM:=EPS;"IF" BNORM=0 "THEN" BNORM:=EPS;
EPSA:=EPS*ANORM;EPSB:=EPS*BNORM;
"FOR" M:=N,M "WHILE" M>=3 "DO"
"BEGIN"
"FOR" I:=M+1,I=1 "WHILE"("IF" I>1 "THEN"ABS(A[I,I-1])>EPSA "ELSE"
"FALSE") "DO" Q:=I-1;
"IF" Q>1 "THEN" A[Q,Q-1]:=0;
L: "IF" Q>=M-1 "THEN" M:=Q-1 "ELSE"
"BEGIN"
"IF" ABS(B[Q,Q])<=EPSB "THEN"
"BEGIN" B[Q,Q]:=0;Q1:=Q+1;
      HSH2COL(Q,Q,M,Q,A[Q,Q],A[Q1,Q],A,B);A[Q1,Q]:=0;
      Q:=Q1;"GOTO" L
"END" "ELSE" M1:=M-1;Q1:=Q+1;CONST:=0.75;ITER[M]:=ITER[M]+1;
STATIONARY:="IF" ITER[M]=1 "THEN" "TRUE" "ELSE"
ABS(A[M,M-1])>=CONST*OLD1"AND"ABS(A[M-1,M-2])>=CONST*OLD2;
"IF" ITER[M]>30"AND"STATIONARY "THEN"
"BEGIN" "FOR" I:=1 "STEP" 1 "UNTIL" M "DO" ITER[I]:=0;
      "GOTO" OUT
"END";
"IF" ITER[M]=10"AND"STATIONARY "THEN"
"BEGIN" A10:=0;A20:=1;A30:=1.1605
"END" "ELSE"
"BEGIN" B11:=B[Q,Q];B22:="IF" ABS(B[Q1,Q1])<EPSB "THEN"EPSB
      "ELSE" B[Q1,Q1];
      B33:="IF" ABS(B[M1,M1])<EPSB "THEN" EPSB "ELSE" B[M1,M1];
"COMMENT"

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B44:= "IF" ABS(B[M,M]) < EPSB "THEN" EPSB "ELSE" B[M,M] ;
A11:= A[Q,Q]/B11; A12:= A[Q,Q1]/B22; A21:= A[Q1,Q]/B11;
A22:= A[Q1,Q1]/B22; A33:= A[M1,M1]/B33; A34:= A[M1,M]/B44;
A43:= A[M,M1]/B33; A44:= A[M,M]/B44; B12:= B[Q,Q1]/B22;
B34:= B[M1,M]/B44;
A10:= ((A33-A11)*(A44-A11)-A34*A43+A43*B34*A11)/A21
      +A12-A11*B12;
A20:= (A22-A11-A21*B12)-(A33-A11)-(A44-A11)+A43*B34;
A30:= A[Q+2,Q1]/B22
"END"; OLD1:= ABS(A[M,M-1]); OLD2:= ABS(A[M-1,M-2]);
"FOR" K:= Q "STEP" 1 "UNTIL" M1 "DO"
"BEGIN" K1:= K+1; K2:= K+2; K3:= "IF" K+3 > M "THEN" M "ELSE" K+3;
KM1:= "IF" K-1 < Q "THEN" Q "ELSE" K-1;
"IF" K = M1 "THEN"
"BEGIN" "IF" K = Q "THEN"
"BEGIN"
HSH3COL(KM1, KM1, M, K, A[K, KM1], A[K1, KM1], A[K2, KM1], A, B);
A[K1, KM1] := A[K2, KM1] := 0
"END";
HSH3ROW2(Q, Q, K3, K, B[K2, K2], B[K2, K1], B[K2, K], A, B);
B[K2, K1] := B[K2, K1] := 0 ;
"END" "ELSE"
"BEGIN" HSH2COL(KM1, KM1, M, K, A[K, KM1], A[K1, KM1], A, B);
A[K1, KM1] := 0
"END";
HSH2ROW2(Q, Q, K3, K3, K, B[K1, K1], B[K1, K], A, B); B[K1, K] := 0
"END"
"END";
OUT;
"END"
"END" QZIT;

"PROCEDURE" QZVAL(N, A, B, EPSA, EPSB, ALFR, ALFI, BETA); "VALUE" N;
"REAL" EPSA, EPSB; "INTEGER" N; "ARRAY" ALFR, ALFI, BETA, A, B;
"BEGIN" "INTEGER" M, L, J; "REAL" AN, BN, A11, A12, A21, A22, B11, B12, B22, E, C, D,
ER, EI, A11R, A11I, A12R, A12I, A21R, A21I, A22R, A22I, CZ, SZR, SZI,
CQ, SQR, SQI, SSR, SSI, TR, TI, BDR, BDI, R;
"FOR" M:= N, M "WHILE" M > 0 "DO"
"IF" ("IF" M > 1 "THEN" A[M, M-1] = 0 "ELSE" "TRUE") "THEN"
"BEGIN" ALFR[M] := A[M, M]; BETA[M] := B[M, M]; ALFI[M] := 0; M := M-1
"END" "ELSE"
"BEGIN" L := M-1; "IF" ABS(B[L, L]) < EPSB "THEN"
"BEGIN" B[L, L] := 0; HSH2COL(L, L, N, L, A[L, L], A[N, L], A, B);
A[M, L] := B[M, L] := 0; ALFR[L] := A[L, L]; ALFR[M] := A[M, M];
BETA[L] := B[L, L]; BETA[M] := B[M, M]; ALFI[M] := ALFI[L] := 0;
"END" "ELSE" "IF" ABS(B[M, M]) < EPSB "THEN"
"BEGIN" B[M, M] := 0; HSH2ROW2(1, 1, M, M, L, A[M, M], A[M, L], A, B);
A[M, L] := B[M, L] := 0; ALFR[L] := A[L, L]; ALFR[M] := A[M, M];
BETA[L] := B[L, L]; BETA[M] := B[M, M]; ALFI[M] := ALFI[L] := 0;
"END" "ELSE"
"BEGIN"
AN := ABS(A[L, L]) + ABS(A[L, M]) + ABS(A[M, L]) + ABS(A[M, M]);
BN := ABS(B[L, L]) + ABS(B[L, M]) + ABS(B[M, M]);
A11 := A[L, L]/AN; A12 := A[L, M]/AN; A21 := A[M, L]/AN; A22 := A[M, M]/AN;
"COMMENT"

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B11:=B[L,L]/BN;B12:=B[L,M]/BN;B22:=B[M,M]/BN;
E:=A11/B11;
C:=(A22-E*B22)/B22-(A21*B12)/(B11*B22)/2;
D:=C*C+(A21*(A12-E*B12))/(B11*B22);
"IF" D>=0 "THEN"
"BEGIN"E:=E+("IF"C<0"THEN"C=SQRT(D)"ELSE"C+SQRT(D));
A11:=A11-E*B11;A12:=A12-E*B12;A22:=A22-E*B22;
"IF" ABS(A11)+ABS(A12)>=ABS(A21)+ABS(A22) "THEN"
HSH2ROW2(1,1,M,M,L,A12,A11,A,B)"ELSE"
HSH2ROW2(1,1,M,M,L,A22,A21,A,B);
"IF"AN>=ABS(E)*BN"THEN"
HSH2COL(L,L,N,L,B[L,L],B[M,L],A,B) "ELSE"
HSH2COL(L,L,N,L,A[L,L],A[M,L],A,B);
A[M,L]:=B[M,L]:=0;
ALFR[L]:=A[L,L];ALFR[M]:=A[M,M];BETA[L]:=B[L,L];
BETA[M]:=B[M,M];ALFI[M]:=ALFI[L]:=0;
"END" "ELSE"
"BEGIN"
ER:=E+C;EI:=SQRT(-D);A11R:=A11-ER*B11;A11I:=EI*B11;
A12R:=A12-ER*B12;A12I:=EI*B12;A21R:=A21;A21I:=0;
A22R:=A22-ER*B22;A22I:=EI*B22;
"IF"ABS(A11R)+ABS(A11I)+ABS(A12R)+ABS(A12I)>=
ABS(A21R)+ABS(A22R)+ABS(A22I)"THEN"
CHSH2(A12R,A12I,-A11R,-A11I,CZ,SZR,SZI)"ELSE"
CHSH2(A22R,A22I,-A21R,-A21I,CZ,SZR,SZI);
"IF"AN>=(ABS(ER)+ABS(EI))*BN"THEN"
CHSH2(CZ*B11+SZR*B12,SZI*B12,SZR*B22,SZI*B22,CQ,SQR,SQI)
"ELSE"CHSH2(CZ*A11+SZR*A12,SZI*A12,CZ*A21+SZR*A22,SZI*A22,
CQ,SQR,SQI);SSR:=SQR*SZR+SQI*SZI;SSI:=SQR*SZI-SQI*SZR;
TR:=CQ*CZ*A11+CQ*SZR*A12+SQR*CZ*A21+SSR*A22;
TI:=CQ*SZI*A12-SQI*CZ*A21+SSI*A22;
BDR:=CQ*CZ*B11+CQ*SZR*B12+SSR*B22;
BDI:=CQ*SZI*B12+SSI*B22;
R:=SQRT(BDR*BDR+BDI*BDI);BETA[L]:=BN*R;
ALFR[L]:=AN*(TR*BDR+TI*BDI)/R;
ALFI[L]:=AN*(TR*BDI-TI*BDR)/R;
TR:=SSR*A11-SQR*CZ*A12-CQ*SZR*A21+CQ*CZ*A22;
TI:=SSI*A11-SQI*CZ*A12+CQ*SZI*A21;
BDR:=SSR*B11-SQR*CZ*B12+CQ*CZ*B22;
BDI:=SSI*B11-SQI*CZ*B12;
R:=SQRT(BDR*BDR+BDI*BDI);BETA[M]:=BN*R;
ALFR[M]:=AN*(TR*BDR+TI*BDI)/R;
ALFI[M]:=AN*(TR*BDI-TI*BDR)/R;
"END"
"END";M:=M-2
"END"
"END" QZVAL;
DWARF:=EM[0];EPS:=EM[1];
HSHDECMUL(N,A,B,DWARF);
HESTGL2(N,A,B);
QZIT(N,A,B,EPS,EPSA,EPSB,ITER);
QZVAL(N,A,B,EPSA,EPSB,ALFR,ALFI,BETA);
"END" QZIVAL;
"EQP"

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"CODE" 34601;
"PROCEDURE" QZI(N,A,B,X,ALFR,ALFI,BETA,ITER,EM);
"VALUE" N;"INTEGER" N;"ARRAY" A,B,X,ALFR,ALFI,BETA,EM;
"INTEGER" "ARRAY" ITER;
"BEGIN" "REAL" DWARF,EPS,EPSA,EPSB;
"REAL" "PROCEDURE" MATMAT(L,U,I,J,A,B);"CODE" 34013;
"PROCEDURE" HSHDECMUL(N,A,B,DWARF);"CODE" 34602;
"PROCEDURE" HESTGL3(N,A,B,X);"CODE" 34603;
"PROCEDURE" HSH2ROW3(L,UA,UB,UX,J,A1,A2,A,B,X);"CODE" 34607;
"PROCEDURE" HSH3ROW3(L,U,UX,J,A1,A2,A3,A,B,X);"CODE" 34609;
"PROCEDURE" HSH2COL(LA,LB,U,I,A1,A2,A,B);"CODE" 34605;
"PROCEDURE" HSH3COL(LA,LB,U,I,A1,A2,A3,A,B);"CODE" 34606;
"PROCEDURE" CHSH2(A1R,A1I,A2R,A2I,C,SR,SI);"CODE" 34611;
"PROCEDURE" COMDIV(XR,XI,YR,YI,ZR,ZI);"CODE" 34342;
"PROCEDURE" QZIT(N,A,B,X,EPS,EPSA,EPSB,ITER);"VALUE" N, EPS;
"REAL" EPS, EPSA, EPSB; "INTEGER" N; "INTEGER" "ARRAY" ITER; "ARRAY" A, B, X;
"BEGIN" "REAL" ANORM, BNORM, ANI, BNI, CONST, A10, A20, A30, B11,
      B22, B33, B44, A11, A12, A21, A22, A33, A34, A43, A44, B12, B34, OLD1, OLD2;
"INTEGER" I, Q, M, M1, Q1, J, K, K1, K2, K3, KM1; "BOOLEAN" STATIONARY;
ANORM:=BNORM:=0; "FOR" I:=1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" BNI:=0; ITER[I]:=0; ANI:= "IF" I>1 "THEN" ABS(A[I,I-1]) "ELSE" 0;
      "FOR" J:=I "STEP" 1 "UNTIL" N "DO"
      "BEGIN" ANI:=ANI+ABS(A[I,J]); BNI:=BNI+ABS(B[I,J])
      "END"; "IF" ANI>ANORM "THEN" ANORM:=ANI; "IF" BNI>BNORM "THEN"
      BNORM:=BNI
"END"; "IF" ANORM=0 "THEN" ANORM:=EPS; "IF" BNORM=0 "THEN" BNORM:=EPS;
EPSA:=EPS*ANORM; EPSB:=EPS*BNORM;
"FOR" M:=N, M "WHILE" M>=3 "DO"
"BEGIN"
"FOR" I:=M+1, I=1 "WHILE" ("IF" I>1 "THEN" ABS(A[I,I-1])>EPSA "ELSE"
"FALSE") "DO" Q:=I-1;
"IF" Q>1 "THEN" A[Q,Q-1]:=0;
L: "IF" Q>=M-1 "THEN" M:=Q-1 "ELSE"
"BEGIN"
"IF" ABS(B[Q,Q])<=EPSB "THEN"
"BEGIN" B[Q,Q]:=0; Q1:=Q+1;
      HSH2COL(Q,Q,N,Q,A[Q,Q],A[Q1,Q],A,B); A[Q1,Q]:=0;
      Q:=Q1; "GOTO" L
"END" "ELSE" M1:=M-1; Q1:=Q+1; CONST:=0.75; ITER[M]:=ITER[M]+1;
STATIONARY:= "IF" ITER[M]=1 "THEN" "TRUE" "ELSE"
ABS(A[M,M-1])>=CONST*OLD1 "AND" ABS(A[M-1,M-2])>=CONST*OLD2;
"IF" ITER[M]>30 "AND" STATIONARY "THEN"
"BEGIN" "FOR" I:=1 "STEP" 1 "UNTIL" M "DO" ITER[I]:=0;
      "GOTO" OUT
"END";
"IF" ITER[M]=10 "AND" STATIONARY "THEN"
"BEGIN" A10:=0; A20:=1; A30:=1.1605
"END" "ELSE"
"BEGIN" B11:=B[Q,Q]; B22:= "IF" ABS(B[Q1,Q1])<EPSB "THEN" EPSB
      "ELSE" B[Q1,Q1];

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"COMMENT"



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B33:= "IF" ABS(B[M1,M1]) < EPSB "THEN" EPSB "ELSE" B[M1,M1];
B44:= "IF" ABS(B[M,M]) < EPSB "THEN" EPSB "ELSE" B[M,M];
A11:= A[Q,Q]/B11; A12:= A[Q,Q1]/B22; A21:= A[Q1,Q]/B11;
A22:= A[Q1,Q1]/B22; A33:= A[M1,M1]/B33; A34:= A[M1,M]/B44;
A43:= A[M,M1]/B33; A44:= A[M,M]/B44; B12:= B[Q,Q1]/B22;
B34:= B[M1,M]/B44;
A10:= ((A33-A11)*(A44-A11)-A34*A43+A43*B34*A11)/A21
      +A12-A11*B12;
A20:= (A22-A11-A21*B12)-(A33-A11)-(A44-A11)+A43*B34;
A30:= A[Q+2,Q1]/B22
"END"; OLD1:= ABS(A[M,M-1]); OLD2:= ABS(A[M-1,M-2]);
"FOR" K:=Q "STEP" 1 "UNTIL" M1 "DO"
"BEGIN" K1:=K+1; K2:=K+2; K3:= "IF" K+3 > M "THEN" M "ELSE" K+3;
KM1:= "IF" K=1 < Q "THEN" Q "ELSE" K-1;
"IF" K = M1 "THEN"
"BEGIN" "IF" K = Q "THEN"
      HSH3COL(KM1, KM1, N, K, A10, A20, A30, A, B) "ELSE"
      "BEGIN"
      HSH3COL(KM1, KM1, N, K, A[K, KM1], A[K1, KM1], A[K2, KM1], A, B);
      A[K1, KM1] := A[K2, KM1] := 0;
      "END";
      HSH3ROW3(1, K3, N, K, B[K2, K2], B[K2, K1], B[K2, K], A, B, X);
      B[K2, K1] := B[K2, K1] := 0;
"END" "ELSE"
"BEGIN" HSH2COL(KM1, KM1, N, K, A[K, KM1], A[K1, KM1], A, B);
      A[K1, KM1] := 0;
"END";
HSH2ROW3(1, K3, K3, N, K, B[K1, K1], B[K1, K], A, B, X); B[K1, K] := 0;
"END"
"END"
"END"; OUT:
"END" QZIT;
"PROCEDURE" QZVAL(N, A, B, X, EPSA, EPSB, ALFR, ALFI, BETA); "VALUE" N;
"REAL" EPSA, EPSB; "INTEGER" N; "ARRAY" ALFR, ALFI, BETA, A, B, X;
"BEGIN" "INTEGER" M, L, J; "REAL" AN, BN, A11, A12, A21, A22, B11, B12, B22, E, C, D,
ER, EI, A11R, A11I, A12R, A12I, A21R, A21I, A22R, A22I, CZ, SZR, SZI,
CQ, SQR, SQI, SSR, SSI, TP, TI, BDR, BDI, R;
"FOR" M:=N, M "WHILE" M > 0 "DO"
"IF" ("IF" M > 1 "THEN" A[M, M-1] = 0 "ELSE" "TRUE") "THEN"
"BEGIN" ALFR[M] := A[M, M]; BETA[M] := B[M, M]; ALFI[M] := 0; M := M-1;
"END" "ELSE"
"BEGIN" L:=M-1; "IF" ABS(B[L, L]) < EPSB "THEN"
"BEGIN" B[L, L] := 0; HSH2COL(L, L, N, L, A[L, L], A[M, L], A, B);
      A[M, L] := B[M, L] := 0; ALFR[L] := A[L, L]; ALFR[M] := A[M, M];
      BETA[L] := B[L, L]; BETA[M] := B[M, M]; ALFI[M] := ALFI[L] := 0;
"END" "ELSE" "IF" ABS(B[M, M]) < EPSB "THEN"
"BEGIN" B[M, M] := 0; HSH2ROW3(1, M, M, N, L, A[M, M], A[M, L], A, B, X);
      A[M, L] := B[M, L] := 0; ALFR[L] := A[L, L]; ALFR[M] := A[M, M];
      BETA[L] := B[L, L]; BETA[M] := B[M, M]; ALFI[M] := ALFI[L] := 0;
"END" "ELSE"
"BEGIN"
AN:= ABS(A[L, L]) + ABS(A[L, M]) + ABS(A[M, L]) + ABS(A[M, M]);
"COMMENT"

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BN:=ABS(B[L,L])+ABS(B[L,M])+ABS(B[M,M]);
A11:=A[L,L]/AN;A12:=A[L,M]/AN;A21:=A[M,L]/AN;A22:=A[M,M]/AN;
B11:=B[L,L]/BN;B12:=B[L,M]/BN;B22:=B[M,M]/BN;
E:=A11/B11;
C:=(A22-E*B22)/B22=(A21*B12)/(B11*B22)/2;
D:=C*C+(A21*(A12-E*B12))/(B11*B22);
"IF" D>=0 "THEN"
"BEGIN"E:=E+("IF"C<0"THEN"C=SQRT(D)"ELSE"C+SQRT(D));
A11:=A11-E*B11;A12:=A12-E*B12;A22:=A22-E*B22;
"IF" ABS(A11)+ABS(A12)>=ABS(A21)+ABS(A22) "THEN"
HSH2ROW3(1,M,M,N,L,A12,A11,A,B,X)"ELSE"
HSH2ROW3(1,M,M,N,L,A22,A21,A,B,X);
"IF"AN>=ABS(E)*BN"THEN"
HSH2COL(L,L,N,L,B[L,L],B[M,L],A,B)"ELSE"
HSH2COL(L,L,N,L,A[L,L],A[M,L],A,B);
A[M,L]:=B[M,L];=0;
ALFR[L]:=A[L,L];ALFR[M]:=A[M,M];BETA[L]:=B[L,L];
BETA[M]:=B[M,M];ALFI[M]:=ALFI[L];=0;
"END""ELSE"
"BEGIN"
ER:=E+C;EI:=SQRT(-D);A11R:=A11-ER*B11;A11I:=EI*B11;
A12R:=A12-ER*B12;A12I:=EI*B12;A21R:=A21;A21I:=0;
A22R:=A22-ER*B22;A22I:=EI*B22;
"IF"ABS(A11R)+ABS(A11I)+ABS(A12R)+ABS(A12I)>=
ABS(A21R)+ABS(A22R)+ABS(A22I)"THEN"
CHSH2(A12R,A12I,-A11R,-A11I,CZ,SZR,SZI)"ELSE"
CHSH2(A22R,A22I,-A21R,-A21I,CZ,SZR,SZI);
"IF"AN>=(ABS(ER)+ABS(EI))*BN"THEN"
CHSH2(CZ*B11+SZR*B12,SZI*B12,SZR*B22,SZI*B22,CQ,SQR,SQI)
"ELSE"CHSH2(CZ*A11+SZR*A12,SZI*A12,CZ*A21+SZR*A22,SZI*A22,
CQ,SQR,SQI);SSR:=SQR*SZR+SQI*SZI;SSI:=SQR*SZI-SQI*SZR;
TR:=CQ*CZ*A11+CQ*SZR*A12+SQR*CZ*A21+SSR*A22;
TI:=CQ*SZI*A12-SQI*CZ*A21+SSI*A22;
BDR:=CQ*CZ*B11+CQ*SZR*B12+SSR*B22;
BDI:=CQ*SZI*B12+SSI*B22;
R:=SQRT(BDR*BDR+BDI*BDI);BETA[L]:=BN*R;
ALFR[L]:=AN*(TR*BDR+TI*BDI)/R;
ALFI[L]:=AN*(TR*BDI-TI*BDR)/R;
TR:=SSR*A11-SQR*CZ*A12-CQ*SZR*A21+CQ*CZ*A22;
TI:=SSI*A11-SQI*CZ*A12+CQ*SZI*A21;
BDR:=SSR*B11-SQR*CZ*B12+CQ*CZ*B22;
BDI:=SSI*B11-SQI*CZ*B12;
R:=SQRT(BDR*BDR+BDI*BDI);BETA[M]:=BN*R;
ALFR[M]:=AN*(TR*BDR+TI*BDI)/R;
ALFI[M]:=AN*(TR*BDI-TI*BDR)/R;
"END"
"END";M:=M-2
"END"
"END" QZVAL

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```

"PROCEDURE" QZVEC(N,A,B,X,EPSA,EPSB,ALFR,ALFI,BETA); "VALUE" N,EPSA,EPSB;
"INTEGER" N;"REAL" EPSA,EPSB;"ARRAY" A,B,ALFR,ALFI,BETA,X;
"BEGIN" "INTEGER" M,MR,MI,L,L1,J,K;"REAL" BETM,ALFM,SL,SK,D,TKK,TKL,TLK,
TLL,ALMI,ALMR,TR,TI,SLR,SLI,SKR,SKI,DR,DI,TKKR,TKKI,TKLR,TKLI,TLKR,
TLKI,TLLR,TLLI,S,R;
"FOR" M:=N "STEP" =1 "UNTIL" 1 "DO"
"IF" ALFI[M]=0 "THEN"
"BEGIN" "COMMENT" M=TH REAL VECTOR;
ALFM:=ALFR[M];BETM:=BETA[M];B[M,M]:=1;L1:=M;
"FOR" L:=M-1 "STEP" =1 "UNTIL" 1 "DO"
"BEGIN" SL:=0;
"FOR" J:=L1 "STEP" 1 "UNTIL" M "DO"
SL:=SL+(BETM*A[L,J]-ALFM*B[L,J])*B[J,M];
"IF" ("IF" L=1 "THEN" BETM*A[L,L-1]=0 "ELSE" "TRUE") "THEN"
"BEGIN" "COMMENT" 1=1 BLOCK;
D:=BETM*A[L,L]-ALFM*B[L,L];
"IF" D=0 "THEN" D:=(EPSA+EPSB)/2;B[L,M]:=SL/D
"END" "ELSE"
"BEGIN" "COMMENT" 2=2 BLOCK;K:=L-1;SKI:=0;
"FOR" J:=L1 "STEP" 1 "UNTIL" M "DO"
SK:=SK+(BETM*A[K,J]-ALFM*B[K,J])*B[J,M];
TKK:=BETM*A[K,K]-ALFM*B[K,K];
TKL:=BETM*A[K,L]-ALFM*B[K,L];
TLK:=BETM*A[L,K];
TLL:=BETM*A[L,L]-ALFM*B[L,L];
D:=TKK*TLL-TKL*TLK;"IF" D=0 "THEN" D:=(EPSA+EPSB)/2;
B[L,M]:= (TLK*SK-TKK*SL)/D;
B[K,M]:= "IF" ABS(TKK)>ABS(TLK) "THEN" -(SK+TKL*B[L,M])/TKK
"ELSE" -(SL+TLL*B[L,M])/TLK;L:=L-1
"END";L1:=L
"END"
"END" "ELSE"
"BEGIN" "COMMENT" COMPLEX VECTOR;
ALMR:=ALFR[M-1];ALMI:=ALFI[M-1];BETM:=BETA[M-1];MR:=M-1;MI:=M;
B[M-1,MR]:=ALMI*B[M,M]/(BETM*A[M,M-1]);
B[M-1,MI]:= (BETM*A[M,M]-ALMR*B[M,M])/(BETM*A[M,M-1]);
B[M,MR]:=0;B[M,MI]:=1;L1:=M-1;
"FOR" L:=M-2 "STEP" =1 "UNTIL" 1 "DO"
"BEGIN" SLR:=SLI:=0;
"FOR" J:=L1 "STEP" 1 "UNTIL" M "DO"
"BEGIN" TR:=BETM*A[L,J]-ALMR*B[L,J];
TI:=ALMI*B[L,J];
SLR:=SLR+TR*B[J,MR]-TI*B[J,MI];
SLI:=SLI+TR*B[J,MI]+TI*B[J,MR]
"END";
"COMMENT"

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```

"IF" ("IF" L = 1 "THEN" BETM * A [L, L-1] = 0 "ELSE" "TRUE") "THEN"
"BEGIN" DR := BETM * A [L, L] - ALMR * B [L, L];
      DI := ALMI * B [L, L];
      COMDIV (-SLR, -SLI, DR, DI, B [L, MR], B [L, MI]);
"END" "ELSE"
"BEGIN" K := L-1; SKR := SKI := 0;
      "FOR" J := L1 "STEP" 1 "UNTIL" M "DO"
      "BEGIN" TR := BETM * A [K, J] - ALMR * B [K, J];
            TI := ALMI * B [K, J];
            SKR := SKR + TR * B [J, MR] - TI * B [J, MI];
            SKI := SKI + TR * B [J, MI] + TI * B [J, MR]
      "END";
      TKKR := BETM * A [K, K] - ALMR * B [K, K];
      TKKI := ALMI * B [K, K];
      TKLR := BETM * A [K, L] - ALMR * B [K, L];
      TKLI := ALMI * B [K, L];
      TLKR := BETM * A [L, K]; TLKI := 0;
      TLLR := BETM * A [L, L] - ALMR * B [L, L];
      TLLI := ALMI * B [L, L];
      DR := TKKR * TLLR - TKKI * TLLI - TKLR * TLKR;
      DI := TKKR * TLLI + TKKI * TLLR - TKLI * TLKR;
      "IF" DR = 0 "AND" DI = 0 "THEN" DR := (EPSA + EPSB) / 2;
      COMDIV (TLKR * SKR - TKKR * SLR + TKKI * SLI, TLKR * SKI - TKKR * SLI -
      TKKI * SLR, DR, DI, B [L, MR], B [L, MI]);
      "IF" ABS (TKKR) + ABS (TKKI) > ABS (TLKR) "THEN"
      COMDIV (-SKR - TKLR * B [L, MR] + TKLI * B [L, MI], -SKI - TKLR * B [L, MI]
      - TKLI * B [L, MR], TKKR, TKKI, B [K, MR], B [K, MI]) "ELSE"
      COMDIV (-SLR - TLLR * B [L, MR] + TLLI * B [L, MI], -SLI - TLLR * B [L, MI]
      - TLLI * B [L, MR], TLKR, TLKI, B [K, MR], B [K, MI]); L := L-1
"END"; L := L
"END"; M := M-1
"END";
"FOR" M := N "STEP" -1 "UNTIL" 1 "DO"
"FOR" K := 1 "STEP" 1 "UNTIL" N "DO"
X [K, M] := MATMAT (1, M, K, M, X, B);
"FOR" M := N "STEP" -1 "UNTIL" 1 "DO"
"BEGIN" S := 0; "IF" ALFI [M] = 0 "THEN"
      "BEGIN" "FOR" K := 1 "STEP" 1 "UNTIL" N "DO"
            "BEGIN" R := ABS (X [K, M]);
                  "IF" R > S "THEN" "BEGIN" S := R; DI := X [K, M] "END"
            "END"; "FOR" K := 1 "STEP" 1 "UNTIL" N "DO"
                  X [K, M] := X [K, M] / D
      "END" "ELSE"
      "BEGIN" "FOR" K := 1 "STEP" 1 "UNTIL" N "DO"
            "BEGIN" R := ABS (X [K, M-1]) + ABS (X [K, M]);
                  R := R * SQRT ((X [K, M-1] / R) ** 2 + (X [K, M] / R) ** 2);
                  "IF" R > S "THEN"
                        "BEGIN" S := R; DR := X [K, M-1]; DI := X [K, M] "END"
            "END"; "FOR" K := 1 "STEP" 1 "UNTIL" N "DO"
                  COMDIV (X [K, M-1], X [K, M], DR, DI, X [K, M-1], X [K, M]); M := M-1
      "END"
"END"
"END"
"END" QZVEC;

```

SECTION : 3.4.1.2

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```

DWARF:=EM[0];EPS:=EM[1];
HSHDECMUL(N,A,B,DWARF);
HESTGL3(N,A,B,X);
QZIT(N,A,B,X,EPS,EPSA,EPSB,ITER);
QZVAL(N,A,B,X,EPSA,EPSB,ALFR,ALFI,BETA);
QZVEC(N,A,B,X,EPSA,EPSB,ALFR,ALFI,BETA)
"END" QZI;
      "EOP"

```

```

"CODE" 34602;
"PROCEDURE" HSHDECMUL(N,A,B,DWARF);"VALUE" N,DWARF;"INTEGER" N;
"REAL" DWARF;"ARRAY" A,B;
"BEGIN" "ARRAY" V[1:N];"INTEGER" J,K,K1,N1;"REAL" R,T,C;
      "REAL" "PROCEDURE" TAMMAT(L,U,I,J,A,B);"CODE" 34014;
      "PROCEDURE" HSHVECMAT(LR,UR,LC,UC,X,U,A);"CODE" 31070;
      K:=1;N1:=N+1;
      "FOR" K1:=2 "STEP" 1 "UNTIL" N1 "DO"
      "BEGIN" R:=TAMMAT(K1,N,K,K,B,B);
            "IF" R>DWARF "THEN"
            "BEGIN" R:= "IF" B[K,K]<0 "THEN" =SQRT(R+B[K,K]*B[K,K])
                  "ELSE" SQRT(R+B[K,K]*B[K,K]);T:=B[K,K]+R;C:=T/R;
                  B[K,K]:=R;V[K]:=1;
                  "FOR" J:=K1 "STEP" 1 "UNTIL" N "DO" V[J]:=B[J,K]/T;
                  HSHVECMAT(K,N,K1,N,C,V,B);HSHVECMAT(K,N,1,N,C,V,A)
            "END";K:=K1
      "END"
"END" HSHDECMUL;
      "EOP"

```

```

"CODE" 34603;
"PROCEDURE" HESTGL3(N,A,B,X);"VALUE" N;"INTEGER" N;"ARRAY" A,B,X;
"BEGIN" "INTEGER" NM1,K,L,K1,L1;
      "PROCEDURE" HSH2COL(LA,LB,U,I,A1,A2,A,B);"CODE" 34605;
      "PROCEDURE" HSH2ROW3(L,UA,UB,UX,J,A1,A2,A,B,X);"CODE" 34607;
      "IF" N>2 "THEN"
      "BEGIN" "FOR" K:=2 "STEP" 1 "UNTIL" N "DO"
            "FOR" L1:=1 "STEP" 1 "UNTIL" K-1 "DO" B[K,L1]:=0;
            NM1:=N-1;K:=1;
            "FOR" K1:=2 "STEP" 1 "UNTIL" NM1 "DO"
            "BEGIN" L1:=N;
                  "FOR" L:=N-1 "STEP" -1 "UNTIL" K1 "DO"
                  "BEGIN"
                        HSH2COL(K,L,N,L,A[L,K],A[L1,K],A,B);A[L1,K]:=0;
                        HSH2ROW3(1,N,L1,N,L,B[L1,L1],B[L1,L],A,B,X);
                        B[L1,L1]:=0;L1:=L
                  "END";K:=K1
            "END"
      "END"
"END" HESTGL3;
      "EOP"

```

```

"CODE" 34604;
"PROCEDURE" HESTGL2(N,A,B); "VALUE" N; "INTEGER" N; "ARRAY" A,B;
"BEGIN" "INTEGER" NM1,K,L,K1,L1;
  "PROCEDURE" HSH2COL(LA,LB,U,I,A1,A2,A,B); "CODE" 34605;
  "PROCEDURE" HSH2ROW2(LA,LB,UA,UB,A1,A2,A,B); "CODE" 34608;
  "IF" N>2 "THEN"
    "BEGIN" "FOR" K:=2 "STEP" 1 "UNTIL" N "DO"
      "FOR" L:=1 "STEP" 1 "UNTIL" K-1 "DO" B[K,L]:=0;
      NM1:=N-1;K:=1;
      "FOR" K1:=2 "STEP" 1 "UNTIL" NM1 "DO"
        "BEGIN" L1:=N;
          "FOR" L:=N-1 "STEP" -1 "UNTIL" K1 "DO"
            "BEGIN"
              HSH2COL(K,L,N,L,A[L,K],A[L1,K],A,B);A[L1,K]:=0;
              HSH2ROW2(1,1,N,L1,L,B[L1,L1],B[L1,L],A,B);
              B[L1,L1]:=0;L1:=L
            "END";K:=K1
          "END"
        "END"
      "END"
    "END" HESTGL2;
  "EOP"

```

```

"CODE" 34605;
"PROCEDURE" HSH2COL(LA,LB,U,I,A1,A2,A,B); "VALUE" LA,LB,U,I,A1,A2;
"INTEGER" LA,LB,U,I; "REAL" A1,A2; "ARRAY" A,B;
"IF" A2=0 "THEN"
"BEGIN" "REAL" R,T,C; "ARRAY" V[I:I+1];
  "PROCEDURE" HSHVECMAT(LR,UR,LC,UC,X,U,A); "CODE" 31070;
  R:= "IF" A1<0 "THEN" -SQRT(A1*A1+A2*A2) "ELSE" SQRT(A1*A1+A2*A2);
  T:=A1+R;C:=T/R;V[I]:=1;V[I+1]:=A2/T;
  HSHVECMAT(I,I+1,LA,U,C,V,A);HSHVECMAT(I,I+1,LB,U,C,V,B)
"END" HSH2COL;
"EOP"

```

```

"CODE" 34606;
"PROCEDURE" HSH3COL(LA,LB,U,I,A1,A2,A3,A,B);
"VALUE" LA,LB,U,I,A1,A2,A3; "INTEGER" LA,LB,I,U; "REAL" A1,A2,A3; "ARRAY" A,B;
"IF" A2=0 "OR" A3=0 "THEN"
"BEGIN" "REAL" R,T,C; "ARRAY" V[I:I+2];
  "PROCEDURE" HSHVECMAT(LR,UR,LC,UC,X,U,A); "CODE" 31070;
  R:= "IF" A1<0 "THEN" -SQRT(A1*A1+A2*A2+A3*A3)
  "ELSE" SQRT(A1*A1+A2*A2+A3*A3);
  T:=A1+R;C:=T/R;V[I]:=1;V[I+1]:=A2/T;V[I+2]:=A3/T;
  HSHVECMAT(I,I+2,LA,U,C,V,A);HSHVECMAT(I,I+2,LB,U,C,V,B)
"END" HSH3COL;
"EOP"

```

```

"CODE" 34607;
"PROCEDURE" HSH2ROW3(L,UA,UB,UX,J,A1,A2,A,B,X); "VALUE" L,UA,UB,UX,
J,A1,A2;"INTEGER" L,UA,UB,UX,J;"REAL" A1,A2;"ARRAY" A,B,X;
"IF" A2#0 "THEN"
"BEGIN" "REAL" R,T,C;"INTEGER" K;"ARRAY" V[J;J+1];
  "PROCEDURE" HSHVECTAM(LR,UR,LC,UC,X,U,A); "CODE" 31073;
  R:="IF" A1<0 "THEN" -SQRT(A1*A1+A2*A2) "ELSE" SQRT(A1*A1+A2*A2);
  T:=A1+R;C:=-T/R;V[J+1]:=1;V[J]:=A2/T;
  HSHVECTAM(L,UA,J,J+1,C,V,A);HSHVECTAM(L,UB,J,J+1,C,V,B);
  HSHVECTAM(1,UX,J,J+1,C,V,X)
"END" HSH2ROW3;
      "EOP"

```

```

"CODE" 34608;
"PROCEDURE" HSH2ROW2(LA,LB,UA,UB,J,A1,A2,A,B); "VALUE" LA,LB,UA,UB,
J,A1,A2;"INTEGER" LA,LB,UA,UB,J;"REAL" A1,A2;"ARRAY" A,B;
"IF" A2#0 "THEN"
"BEGIN" "REAL" R,T,C;"INTEGER" K;"ARRAY" V[J;J+1];
  "PROCEDURE" HSHVECTAM(LR,UR,LC,UC,X,U,A); "CODE" 31073;
  R:="IF" A1<0 "THEN" -SQRT(A1*A1+A2*A2) "ELSE" SQRT(A1*A1+A2*A2);
  T:=A1+R;C:=-T/R;V[J+1]:=1;V[J]:=A2/T;
  HSHVECTAM(LA,UA,J,J+1,C,V,A);HSHVECTAM(LB,UB,J,J+1,C,V,B)
"END" HSH2ROW2;
      "EOP"

```

```

"CODE" 34609;
"PROCEDURE" HSH3ROW3(L,U,UX,J,A1,A2,A3,A,B,X);
"VALUE" L,U,UX,J,A1,A2,A3;"INTEGER" L,J,U,UX;"REAL" A1,A2,A3;"ARRAY" A,B,X;
"IF" A2#0 "OR" A3#0 "THEN"
"BEGIN" "REAL" R,T,C;"ARRAY" V[J;J+2];"INTEGER" K;
  "PROCEDURE" HSHVECTAM(LR,UR,LC,UC,X,U,A); "CODE" 31073;
  R:="IF" A1<0 "THEN" -SQRT(A1*A1+A2*A2+A3*A3)
  "ELSE" SQRT(A1*A1+A2*A2+A3*A3);
  T:=A1+R;C:=-T/R;V[J+2]:=1;V[J+1]:=A2/T;V[J]:=A3/T;
  HSHVECTAM(L,U,J,J+2,C,V,A);HSHVECTAM(L,U,J,J+2,C,V,B);
  HSHVECTAM(L,UX,J,J+2,C,V,X)
"END" HSH3ROW3;
      "EOP"

```

```

"CODE" 34610;
"PROCEDURE" HSH3ROW2(LA,LB,U,J,A1,A2,A3,A,B);
"VALUE" LA,LB,U,J,A1,A2,A3;"INTEGER" LA,LB,U,J;"REAL" A1,A2,A3;"ARRAY" A,B;
"IF" A2#0 "OR" A3#0 "THEN"
"BEGIN" "REAL" R,T,C;"ARRAY" V[J;J+2];
  "PROCEDURE" HSHVECTAM(LR,UR,LC,UC,X,U,A); "CODE" 31073;
  R:="IF" A1<0 "THEN" -SQRT(A1*A1+A2*A2+A3*A3)
  "ELSE" SQRT(A1*A1+A2*A2+A3*A3);
  T:=A1+R;C:=-T/R;V[J+2]:=1;V[J+1]:=A2/T;V[J]:=A3/T;
  HSHVECTAM(LA,U,J,J+2,C,V,A);HSHVECTAM(LB,U,J,J+2,C,V,B)
"END" HSH3ROW2;
      "EOP"

```

1-st REVISION, 1975



SECTION : 3.5.1.1

(DECEMBER 1975)

PAGE 1

AUTHORS : G.H.GOLUB AND C.REINSCH

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BRIEF DESCRIPTION :

THIS SECTION CONTAINS TWO PROCEDURES, QRISNGVALBID AND QRISNGVALDEC BID. BOTH PROCEDURES CALCULATE THE SINGULAR VALUES OF A BIDIAGONAL MATRIX. MOREOVER, THE SECOND PROCEDURE CALCULATES THE SINGULAR VALUES DECOMPOSITION OF A FULL MATRIX OF WHICH THE BIDIAGONAL AND THE PRE- AND POSTMULTIPLYING MATRICES, AS CALCULATED BY HSHREABID ARE GIVEN.

KEYWORDS :

SINGULAR VALUES  
QR ITERATION  
BIDIAGONAL MATRICES



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SUBSECTION : QRISNGVALBID

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"INTEGER" "PROCEDURE" QRISNGVALBID(D, B, N, EM);

"VALUE" N; "INTEGER" N; "ARRAY" D, B, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

D: <ARRAY IDENTIFIER>;

"ARRAY" D[1:N];

ENTRY: THE DIAGONAL OF THE BIDIAGONAL MATRIX;

EXIT: THE SINGULAR VALUES;

B: <ARRAY IDENTIFIER>;

"ARRAY" B[1:N];

ENTRY: THE SUPER DIAGONAL OF THE BIDIAGONAL MATRIX, IN B[1:N-1];

N: <ARITHMETIC EXPRESSION>;

THE LENGTH OF B AND D;

EM: <ARRAY IDENTIFIER>;

"ARRAY" EM[1:7];

ENTRY: EM[1]: THE INFINITY NORM OF THE MATRIX;

EM[2]: THE RELATIVE PRECISION IN THE SINGULAR VALUES;

EM[4]: THE MAXIMAL NUMBER OF ITERATIONS TO BE PERFORMED;

EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE;

EXIT: EM[3]: THE MAXIMAL NEGLECTED SUPERDIAGONAL ELEMENT;

EM[5]: THE NUMBER OF ITERATIONS PERFORMED;

EM[7]: THE NUMERICAL RANK OF THE MATRIX, I.E. THE NUMBER OF SINGULAR VALUES GREATER THAN OR EQUAL TO EM[6].

MOREOVER :

QRISNGVALBID:= THE NUMBER OF SINGULAR VALUES NOT FOUND, I.E. A NUMBER NOT EQUAL TO ZERO IF THE NUMBER OF ITERATIONS EXCEEDS EM[4].

PROCEDURES USED : NONE

REQUIRED CENTRAL MEMORY : NO AUXILIARY ARRAYS ARE DECLARED

RUNNING TIME :

THE RUNNING TIME DEPENDS STRONGLY UPON THE PROPERTIES OF THE MATRIX

METHOD AND PERFORMANCE :

THE METHOD IS DESCRIBED IN DETAIL IN [1]. THIS PROCEDURE IS A REWRITING OF PART OF THE PROCEDURE SVD PUBLISHED THERE BY G.H.GOLUB AND C.REINSCH.

LANGUAGE : ALGOL 60.

SECTION : 3.5.1.1

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PAGE 3

SUBSECTION : QRISNGVALDECBID

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"INTEGER" "PROCEDURE" QRISNGVALDECBID(D, B, M, N, U, V, EM);

"VALUE" M, N; "INTEGER" M, N; "ARRAY" D, B, U, V, EM;

THE MEANING OF THE FORMAL PARAMETERS IS :

D: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" D[1:N];

ENTRY: THE DIAGONAL OF THE BIDIAGONAL MATRIX;

EXIT: THE SINGULAR VALUES;

B: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" B[1:N];

ENTRY: THE SUPER DIAGONAL OF THE BIDIAGONAL MATRIX, IN B[1:N-1];

M: &lt;ARITHMETIC EXPRESSION&gt;;

THE NUMBER OF ROWS OF THE MATRIX U;

N: &lt;ARITHMETIC EXPRESSION&gt;;

THE LENGTH OF B AND D, THE NUMBER OF COLUMNS OF U AND THE NUMBER OF COLUMNS AND ROWS OF V;

U: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" U[1:M,1:N];

ENTRY: THE PREMULTIPLYING MATRIX AS PRODUCED BY PRETFMMAT (SECTION 3.2.2.1.1);

EXIT: THE PREMULTIPLYING MATRIX U OF THE SINGULAR VALUES DECOMPOSITION  $U * S * V'$ ;

V: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" V[1:N,1:N];

ENTRY: THE TRANSPOSE OF THE POSTMULTIPLYING MATRIX AS PRODUCED BY PSTTFMMAT (SECTION 3.2.2.1.1);

EXIT: THE TRANSPOSE OF THE POSTMULTIPLYING MATRIX V OF THE SINGULAR VALUES DECOMPOSITION;

EM: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" EM[1:7];

ENTRY: EM[1]: THE INFINITY NORM OF THE MATRIX;

EM[2]: THE RELATIVE PRECISION IN THE SINGULAR VALUES;

EM[4]: THE MAXIMAL NUMBER OF ITERATIONS TO BE PERFORMED;

EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE;

EXIT: EM[3]: THE MAXIMAL NEGLECTED SUPERDIAGONAL ELEMENT;

EM[5]: THE NUMBER OF ITERATIONS PERFORMED;

EM[7]: THE NUMERICAL RANK OF THE MATRIX, I.E. THE NUMBER OF SINGULAR VALUES GREATER THAN OR EQUAL TO EM[6].

MOREOVER :

QRISNGVALDECBID:= THE NUMBER OF SINGULAR VALUES NOT FOUND, I.E. A NUMBER NOT EQUAL TO ZERO IF THE NUMBER OF ITERATIONS EXCEEDS EM[4].

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PROCEDURES USED :

ROTCOL = CP34040

REQUIRED CENTRAL MEMORY : NO AUXILIARY ARRAYS ARE DECLARED

RUNNING TIME :

THE RUNNING TIME DEPENDS STRONGLY UPON THE PROPERTIES OF THE MATRIX

METHOD AND PERFORMANCE :

THE METHOD IS DESCRIBED IN DETAIL IN [1]. THIS PROCEDURE IS A REWRITING OF PART OF THE PROCEDURE SVD PUBLISHED THERE BY G.H.GOLUB AND C.REINSCH.

LANGUAGE : ALGOL 60

REFERENCES :

[1] WILKINSON, J.H. AND C.REINSCH  
HANDBOOK OF AUTOMATIC COMPUTATION, VOL. 2  
LINEAR ALGEBRA  
HEIDELBERG (1971)

EXAMPLE OF USE :

FOR AN EXAMPLE OF USE ONE IS REFERRED TO SECTION 3.5.1.2

SOURCE TEXT(S) :

```

"CODE" 34270;
"INTEGER" "PROCEDURE" QRISNGVALBID(D, B, N, EM);
"VALUE" N; "INTEGER" N; "ARRAY" D, B, EM;
"BEGIN" "INTEGER" N1, K, K1, I, I1, COUNT, MAX, RNK;
"REAL" TOL, BMAX, Z, X, Y, G, H, F, C, S, MIN;
TOL:= EM[2] * EM[1]; COUNT:= 0; BMAX:= 0; MAX:= EM[4]; MIN:= EM[6];
RNK:= N;
IN: K:= N; N1:= N - 1;
NEXT: K:= K - 1; "IF" K > 0 "THEN"
"BEGIN" "IF" ABS(B[K]) >= TOL "THEN"
"BEGIN" "IF" ABS(D[K]) >= TOL "THEN" "GOTO" NEXT;
C:= 0; S:= 1;
"FOR" I:= K "STEP" 1 "UNTIL" N1 "DO"
"BEGIN" F:= S * B[I]; B[I]:= C * B[I]; I1:= I + 1;
"IF" ABS(F) < TOL "THEN" "GOTO" NEGLECT;
G:= D[I1]; D[I1]:= H:= SQRT(F * F + G * G);
C:= G / H; S:= - F / H
"END"

```

```

        NEGLECT;
        "END"
        "ELSE" "IF" ABS(B[K]) > BMAX "THEN" BMAX:= ABS(B[K])
"END";
"IF" K = N1 "THEN"
"BEGIN" "IF" D[N] < 0 "THEN" D[N]:= - D[N];
        "IF" D[N] <= MIN "THEN" RNK:= RNK + 1; N:= N1
"END"
"ELSE"
"BEGIN" COUNT:= COUNT + 1; "IF" COUNT > MAX "THEN" "GOTO" END;
        K1:= K + 1; Z:= D[N]; X:= D[K1]; Y:= D[N1];
        G:= "IF" N1 = 1 "THEN" 0 "ELSE" B[N1 - 1]; H:= B[N1];
        F:= ((Y = Z) * (Y + Z) + (G = H) * (G + H)) / (2 * H * Y);
        G:= SQRT(F * F + 1);
        F:= ((X = Z) * (X + Z) + H * (Y / ("IF" F < 0 "THEN" F = G
        "ELSE" F + G) - H)) / X; C:= S:= 1;
        "FOR" I:= K1 + 1 "STEP" 1 "UNTIL" N "DO"
        "BEGIN" I1:= I - 1; G:= B[I1]; Y:= D[I]; H:= S * G; G:= C * G;
                Z:= SQRT(F * F + H * H); C:= F / Z; S:= H / Z;
                "IF" I1 = K1 "THEN" B[I1 - 1]:= Z; F:= X * C + G * S;
                G:= G * C - X * S; H:= Y * S; Y:= Y * C;
                D[I1]:= Z:= SQRT(F * F + H * H); C:= F / Z; S:= H / Z;
                F:= C * G + S * Y; X:= C * Y - S * G
        "END";
        B[N1]:= F; D[N]:= X
"END";
"IF" N > 0 "THEN" "GOTO" IN;
END; EM[3]:= BMAX; EM[5]:= COUNT; EM[7]:= RNK; QRISNGVALBID:= N
"END" QRISNGVALBID;
"EOP"

```

```

"CODE" 34271;

```

```

"INTEGER" "PROCEDURE" QRISNGVALDECBD(D, B, M, N, U, V, EM);

```

```

"VALUE" M, N; "INTEGER" M, N; "ARRAY" D, B, U, V, EM;

```

```

"BEGIN" "INTEGER" NO, N1, K, K1, I, I1, COUNT, MAX, RNK;

```

```

        "REAL" TOL, BMAX, Z, X, Y, G, H, F, C, S, MIN;

```

```

        "PROCEDURE" ROTCOL(L, U, I, J, A, C, S);

```

```

        "VALUE" L, U, I, J, C, S; "INTEGER" L, U, I, J;

```

```

        "REAL" C, S; "ARRAY" A;

```

```

"CODE" 34040; "COMMENT"

```

```

TOL:= EM[2] * EM[1]; COUNT:= 0; BMAX:= 0; MAX:= EM[4]; MIN:= EM[6];
RNK:= NO:= N;
IN: K:= N; N1:= N - 1;
NEXT: K:= K - 1; "IF" K > 0 "THEN"
"BEGIN" "IF" ABS(B[K]) >= TOL "THEN"
"BEGIN" "IF" ABS(D[K]) >= TOL "THEN" "GOTO" NEXT;
C:= 0; S:= 1;
"FOR" I:= K "STEP" 1 "UNTIL" N1 "DO"
"BEGIN" F:= S * B[I]; B[I]:= C * B[I]; I1:= I + 1;
"IF" ABS(F) < TOL "THEN" "GOTO" NEGLECT;
G:= D[I1]; D[I1]:= H:= SQRT(F * F + G * G);
C:= G / H; S:= F / H;
ROTCOL(1, M, K, I1, U, C, S)
"END";
NEGLECT:
"END"
"ELSE" "IF" ABS(B[K]) > BMAX "THEN" BMAX:= ABS(B[K])
"END";
"IF" K = N1 "THEN"
"BEGIN" "IF" D[N] < 0 "THEN"
"BEGIN" D[N]:= - D[N];
"FOR" I:= 1 "STEP" 1 "UNTIL" NO "DO" V[I,N]:= - V[I,N]
"END";
"IF" D[N] <= MIN "THEN" RNK:= RNK + 1; N1:= N1
"END"
"ELSE"
"BEGIN" COUNT:= COUNT + 1; "IF" COUNT >= MAX "THEN" "GOTO" END;
K1:= K + 1; Z:= D[N]; X:= D[K1]; Y:= D[N1];
G:= "IF" N1 = 1 "THEN" 0 "ELSE" B[N1 = 1]; H:= B[N1];
F:= ((Y - Z) * (Y + Z) + (G - H) * (G + H)) / (2 * H * Y);
G:= SQRT(F * F + 1);
F:= ((X - Z) * (X + Z) + H * (Y / ("IF" F < 0 "THEN" F = G
"ELSE" F + G) - H)) / X; C:= S:= 1;
"FOR" I:= K1 + 1 "STEP" 1 "UNTIL" N "DO"
"BEGIN" I1:= I - 1; G:= B[I1]; Y:= D[I]; H:= S * G; G:= C * G;
Z:= SQRT(F * F + H * H); C:= F / Z; S:= H / Z;
"IF" I1 = K1 "THEN" B[I1 = 1]:= Z; F:= X * C + G * S;
G:= G * C - X * S; H:= Y * S; Y:= Y * C;
ROTCOL(1, NO, I1, I, V, C, S);
D[I1]:= Z:= SQRT(F * F + H * H); C:= F / Z; S:= H / Z;
F:= C * G + S * Y; X:= C * Y - S * G;
ROTCOL(1, M, I1, I, U, C, S)
"END";
B[N1]:= F; D[N]:= X
"END";
"IF" N > 0 "THEN" "GOTO" IN;
END: EM[3]:= BMAX; EM[5]:= COUNT; EM[7]:= RNK; QRISNGVALDECIBID:= N
"END" QRISNGVALDECIBID;
"EOF"
    
```

1-st REVISION, 1975



SECTION : 3.5.1.2

(JULY 1974)

PAGE 1

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RECEIVED : 731217

BRIEF DESCRIPTION :

THIS SECTION CONTAINS TWO PROCEDURES, QRISNGVAL AND QRISNGVALDEC.  
QRISNGVAL CALCULATES THE SINGULAR VALUES OF A GIVEN MATRIX.  
QRISNGVALDEC CALCULATES THE SINGULAR VALUES DECOMPOSITION  
 $U * S * V'$ , WITH U AND V ORTHOGONAL AND S POSITIVE DIAGONAL.

KEYWORDS :

SINGULAR VALUES  
QR ITERATION

SECTION : 3.5.1.2

(DECEMBER 1975)

PAGE 2

SUBSECTION : QRISNGVAL

CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"INTEGER" "PROCEDURE" QRISNGVAL(A, M, N, VAL, EM);

"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, VAL, EM;

THE MEANING OF THE FORMAL PARAMETERS IS :

A: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" A[1:M,1:N];

ENTRY: THE INPUT MATRIX;

EXIT: DATA CONCERNING THE TRANSFORMATION TO BIDIAGONAL FORM;

M: &lt;ARITHMETIC EXPRESSION&gt;;

THE NUMBER OF ROWS OF A;

N: &lt;ARITHMETIC EXPRESSION&gt;;

THE NUMBER OF COLUMNS OF A, N SHOULD SATISFY  $N \leq M$ ;

VAL: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" VAL[1:N];

EXIT: THE SINGULAR VALUES;

EM: &lt;ARRAY IDENTIFIER&gt;;

"ARRAY" EM[0:7];

ENTRY: EM[0]: THE MACHINE PRECISION;

EM[2]: THE RELATIVE PRECISION IN THE SINGULAR VALUES;

EM[4]: THE MAXIMAL NUMBER OF ITERATIONS TO BE PERFORMED;

EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE;

EXIT: EM[1]: THE INFINITY NORM OF THE MATRIX;

EM[3]: THE MAXIMAL NEGLECTED SUPERDIAGONAL ELEMENT;

EM[5]: THE NUMBER OF ITERATIONS PERFORMED;

EM[7]: THE NUMERICAL RANK OF THE MATRIX, I.E. THE NUMBER OF SINGULAR VALUES GREATER THAN OR EQUAL TO EM[6].

MOREOVER :

QRISNGVAL := THE NUMBER OF SINGULAR VALUES NOT FOUND, I.E. A NUMBER NOT EQUAL TO ZERO IF THE NUMBER OF ITERATIONS EXCEEDS EM[4].

PROCEDURES USED :

HSHREABID = CP34260

QRISNGVALBID = CP34270

REQUIRED CENTRAL MEMORY : AN AUXILIARY ARRAY OF N REALS IS DECLARED

RUNNING TIME :

THE RUNNING TIME DEPENDS UPON THE PROPERTIES OF THE MATRIX, HOWEVER THE PROCESS OF BIDIAGONALIZATION DOMINATES, AND ITS RUNNING TIME IS PROPORTIONAL TO  $(M + N) * N * N$ 

METHOD AND PERFORMANCE :

THE MATRIX IS FIRST TRANSFORMED TO BIDIAGONAL FORM BY THE PROCEDURE HSHREABID (SECTION 3.2.2.1.1), AND THEN THE SINGULAR VALUES ARE CALCULATED BY QRISNGVALBID (SECTION 3.5.1.1).

LANGUAGE : ALGOL 60

## SUBSECTION : QRISNGVALDEC

## CALLING SEQUENCE :

THE HEADING OF THE PROCEDURE IS :

"INTEGER" "PROCEDURE" QRISNGVALDEC(A, M, N, VAL, V, EM);

"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, VAL, V, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;

"ARRAY" A[1:M,1:N];

ENTRY: THE GIVEN MATRIX;

EXIT: THE MATRIX U IN THE SINGULAR VALUES DECOMPOSITION  
 $U * S * V^T$ ;

M: <ARITHMETIC EXPRESSION>;

THE NUMBER OF ROWS OF A;

N: <ARITHMETIC EXPRESSION>;

THE NUMBER OF COLUMNS OF A, N SHOULD SATISFY  $N \leq M$ ;

VAL: <ARRAY IDENTIFIER>;

"ARRAY" VAL[1:N];

EXIT: THE SINGULAR VALUES;

V: <ARRAY IDENTIFIER>;

"ARRAY" V[1:N,1:N];

EXIT: THE TRANSPOSE OF MATRIX V IN THE SINGULAR VALUES  
 DECOMPOSITION;

EM: <ARRAY IDENTIFIER>;

"ARRAY" EM[0:7];

ENTRY: EM[0]: THE MACHINE PRECISION;

EM[2]: THE RELATIVE PRECISION IN THE SINGULAR VALUES;

EM[4]: THE MAXIMAL NUMBER OF ITERATIONS TO BE PERFORMED;

EM[6]: THE MINIMAL NON-NEGLECTABLE SINGULAR VALUE;

EXIT: EM[1]: THE INFINITY NORM OF THE MATRIX;

EM[3]: THE MAXIMAL NEGLECTED SUPER DIAGONAL ELEMENT;

EM[5]: THE NUMBER OF ITERATIONS PERFORMED;

EM[7]: THE NUMERICAL RANK OF THE MATRIX, I.E. THE NUMBER OF  
 SINGULAR VALUES GREATER THAN OR EQUAL TO EM[6].

MOREOVER :

QRISNGVALDEC:= THE NUMBER OF SINGULAR VALUES NOT FOUND, I.E. A  
 NUMBER NOT EQUAL TO ZERO IF THE NUMBER OF ITERATIONS EXCEEDS  
 EM[4].

PROCEDURES USED :

HSHREABID = CP34260

PSTTFMAT = CP34261

PRETFMAT = CP34262

QRISNGVALDEC BID = CP34271

REQUIRED CENTRAL MEMORY : AN AUXILIARY ARRAY OF N ELEMENTS IS DECLARED



## RUNNING TIME :

THE RUNNING TIME DEPENDS UPON THE PROPERTIES OF THE MATRIX, HOWEVER THE PROCESS OF BIDIAGONALIZATION DOMINATES, AND ITS RUNNING TIME IS PROPORTIONAL TO  $(M + N) * N * N$

## METHOD AND PERFORMANCE:

THE MATRIX IS FIRST TRANSFORMED TO BIDIAGONAL FORM BY THE PROCEDURE HSHREABID (SECTION 3.2.2.1.1), THE TWO TRANSFORMING MATRICES ARE CALCULATED BY THE PROCEDURES PSTTFMMAT AND PRETFMMAT (SECTIONS 3.2.2.1.2 AND 3.2.2.1.3 RESPECTIVELY), AND FINALLY THE SINGULAR VALUES DECOMPOSITION IS CALCULATED BY QRISNGVALDEC (SECTION 3.5.1.1).

## LANGUAGE : ALGOL 60

## REFERENCES :

WILKINSON, J.H. AND C.REINSCH  
HANDBOOK OF AUTOMATIC COMPUTATION, VOL. 2  
LINEAR ALGEBRA  
HEIDELBERG (1971)

## EXAMPLE OF USE :

AS THE PROCEDURE QRISNGVALDEC CALCULATES THE SINGULAR VALUES OF A MATRIX IN EXACTLY THE SAME WAY AS QRISNGVAL, WE GIVE HER ONLY AN EXAMPLE OF USE OF THE PROCEDURE QRISNGVALDEC. FIRST WE GIVE A PROGRAM, AND THEN THE RESULTS OF THIS PROGRAM:

```

"BEGIN" "ARRAY" A[1:6,1:5], V[1:5,1:5], VAL[1:5], EM[0:7];
  "INTEGER" I, J;
  "INTEGER" "PROCEDURE" QRISNGVALDEC(A, M, N, VAL, V, EM);
  "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, VAL, V, EM;
  "CODE" 34273;

  "FOR" I:= 1 "STEP" 1 "UNTIL" 5 "DO"
  "FOR" J:= 1 "STEP" 1 "UNTIL" 5 "DO"
  A[I,J]:= 1 / (I + J - 1);
  EM[0]:= "-14; EM[2]:= "-12; EM[4]:= 25; EM[6]:= "-10;
  I:= QRISNGVALDEC(A, 6, 5, VAL, V, EM);
  OUTPUT(61, "("3B, "("NUMBER SINGULAR VALUES NOT FOUND : """,
  3ZD, /, 3B, "("INFINITY NORM : """, N, /, 3B,
  "("MAX NEGLECTED SUBDIAGONAL ELEMENT : """, N, /, 3B,
  "("NUMBER ITERATIONS : """, 3ZD, /, 3B,
  "("NUMERICAL RANK : """, 3ZD, /""", I, EM[1], EM[3], EM[5],
  EM[7]);
  OUTPUT(61, "("/, 3B, "("SINGULAR VALUES : """, /""");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 5 "DO"
  OUTPUT(61, "("/, 3B, N""", VAL[I]);
  OUTPUT(61, "("/, /, 3B, "("MATRIX U, FIRST 3 COLUMNS""", /""");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 6 "DO"
  OUTPUT(61, "("/, 3B, 3(N)""", A[I,1], A[I,2], A[I,3]);
  OUTPUT(61, "("/, /, 13B, "("LAST 2 COLUMNS""", /""");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 6 "DO"
  OUTPUT(61, "("/, 13B, 2(N)""", A[I,4], A[I,5])
"END"

```

NUMBER SINGULAR VALUES NOT FOUND : 0  
 INFINITY NORM : +2.2833333333334"=+000  
 MAX NEGLECTED SUBDIAGONAL ELEMENT : +5.7786437871158"=014  
 NUMBER ITERATIONS : 5  
 NUMERICAL RANK : 5

SINGULAR VALUES :

+1.5921172587262"=+000  
 +2.2449595426097"=001  
 +1.3610556101029"=002  
 +4.3245382038374"=004  
 +6.4001947134260"=006

MATRIX U, FIRST 3 COLUMNS

=7.5497918208386"=001	+6.1011090790645"=001	=2.3287173869184"=001
=4.3909273679284"=001	=2.2602102994174"=001	+7.0245315582712"=001
=3.1703146681544"=001	=3.7306964696148"=001	+2.1607293656979"=001
=2.4999458583084"=001	=3.9557817833576"=001	=1.4665595223684"=001
=2.0704999076883"=001	=3.8483260608872"=001	=3.6803786187007"=001
=1.7699734614538"=001	=3.6458192866515"=001	=4.9868122801331"=001

LAST 2 COLUMNS

+5.8625326935176"=002	=1.0184205426735"=002
=4.8169088124009"=001	+1.7189132301455"=001
+5.4982292571999"=001	=5.9788920283495"=001
+4.0633053815463"=001	+4.5989617524697"=001
=6.1755991033503"=002	+4.3029765325422"=001
=5.4158416488948"=001	=4.6499203623570"=001

SOURCE TEXT(S):

```

"CODE" 34272;
"INTEGER" "PROCEDURE" QRISNGVAL(A, M, N, VAL, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, VAL, EM;
"BEGIN" "ARRAY" B[1:N];

    "PROCEDURE" HSHREABID(A, M, N, D, B, EM);
    "VALUE" M, N; "INTEGER" M, N; "ARRAY" D, B, EM;
    "CODE" 34260;

    "INTEGER" "PROCEDURE" QRISNGVALBID(D, B, N, EM);
    "VALUE" N; "INTEGER" N; "ARRAY" D, B, EM;
    "CODE" 34270;

    HSHREABID(A, M, N, VAL, B, EM);
    QRISNGVAL:= QRISNGVALBID(VAL, B, N, EM)
"END" QRISNGVAL;
    "EOP"

"CODE" 34273;
"INTEGER" "PROCEDURE" QRISNGVALDEC(A, M, N, VAL, V, EM);
"VALUE" M, N; "INTEGER" M, N; "ARRAY" A, VAL, V, EM;
"BEGIN" "ARRAY" B[1:N];

    "PROCEDURE" HSHREABID(A, M, N, D, B, EM);
    "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, D, B, EM;
    "CODE" 34260;

    "PROCEDURE" PSTTFMMAT(A, N, V, B);
    "VALUE" N; "INTEGER" N; "ARRAY" A, V, B;
    "CODE" 34261;

    "PROCEDURE" PRETFMMAT(A, M, N, D);
    "VALUE" M, N; "INTEGER" M, N; "ARRAY" A, D;
    "CODE" 34262;

    "INTEGER" "PROCEDURE" QRISNGVALDECIBID(D, B, M, N, U, V, EM);
    "VALUE" M, N; "INTEGER" M, N; "ARRAY" D, B, U, V, EM;
    "CODE" 34271;

    HSHREABID(A, M, N, VAL, B, EM);
    PSTTFMMAT(A, N, V, B); PRETFMMAT(A, M, N, VAL);
    QRISNGVALDEC:= QRISNGVALDECIBID(VAL, B, M, N, A, V, EM)
"END" QRISNGVALDEC;
    "EOP"

```

SECTION : 3.6.1

(DECEMBER 1975)

PAGE 1

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RECEIVED: 740327.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS A PROCEDURE TO CALCULATE ALL ZEROS OF A POLYNOMIAL WITH REAL COEFFICIENTS. THIS IS DONE BY MEANS OF THE COMPANION MATRIX.

KEYWORDS:

ZEROS  
REAL POLYNOMIAL  
COMPANION MATRIX

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS :  
"INTEGER" "PROCEDURE" POLZEROS(A, N, EM, RE, IM);  
"VALUE" N; "INTEGER" N; "ARRAY" A, EM, RE, IM;  
"CODE" 34500;

THE MEANING OF THE FORMAL PARAMETERS IS:

A: <ARRAY IDENTIFIER>;

"ARRAY" A[0:N];

ENTRY: THE COEFFICIENTS OF THE POLYNOMIAL, IN SUCH A WAY THAT  
$$P(X) = A[N] * X ** N + A[N-1] * X ** (N-1) + \dots + A[0].$$

EXIT: THE ARRAY ELEMENTS ARE ALTERED.

N: <ARITHMETIC EXPRESSION>;

THE DEGREE OF THE POLYNOMIAL.

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0]: THE MACHINE PRECISION;  
 EM[2]: THE RELATIVE PRECISION FOR THE ZEROS;  
 EM[4]: THE MAXIMAL NUMBER OF ITERATIONS TO BE PERFORMED;  
 EXIT: EM[1]: AN UPPERBOUND FOR THE ZEROS;  
 EM[3]: THE MAXIMAL NEGLECTED SUBDIAGONAL ELEMENT IN THE  
 QR-ITERATION;  
 EM[5]: THE NUMBER OF ITERATIONS PERFORMED; UPON EXIT  
 EM[5] = EM[4] + 1, IFF THE QR-ITERATION DID NOT STOP  
 SUCCESSFULLY.

RE: <ARRAY IDENTIFIER>;  
 "ARRAY" RE[1:N];  
 EXIT: THE REAL PARTS OF THE ZEROS OF THE POLYNOMIAL, IF ONLY K  
 ZEROS ARE FOUND ONLY RE[N-K+1:N] CONTAINS INFORMATION.

IM: <ARRAY IDENTIFIER>;  
 "ARRAY" IM[1:N];  
 EXIT: THE IMAGINARY PARTS OF THE ZEROS OF THE POLYNOMIAL, IN  
 SUCH A WAY THAT THE ZEROS ARE RE[J] + I \* IM[J].

## MOREOVER:

POLZEROS = THE NUMBER OF ZEROS NOT FOUND (I.E. BECAUSE EITHER THE  
 QR-ITERATION DID NOT FINISH SUCCESSFULLY, OR SOME LEADING  
 COEFFICIENTS OF THE POLYNOMIAL WERE 0).

## PROCEDURES USED:

COMVALQRI = CP34190

## REQUIRED CENTRAL MEMORY:

AUXILIARY ARRAYS ARE DECLARED TO A TOTAL OF  $(NZ + 1) * NZ$  REALS,  
 WHERE NZ DENOTES THE NUMBER OF ZEROS NOT EQUAL TO 0.

## RUNNING TIME:

THE EXECUTION TIME DEPENDS STRONGLY UPON THE NUMBER OF ITERATIONS  
 PERFORMED, EACH ITERATION IS ROUGHLY PROPORTIONAL TO N CUBED.

## METHOD AND PERFORMANCE:

WE FIRST DESCRIBE THE STEPS THAT ARE TAKEN IN ORDER TO YIELD AN EQUILIBRATED COMPANION MATRIX. FOUR STEPS ARE INVOLVED IN THIS PROCESS:

1. IF SOME LEADING COEFFICIENTS ARE ZERO, IT IS CLEAR THAT IN FACT WE HAVE NOT GOT A N-TH DEGREE POLYNOMIAL, BUT A POLYNOMIAL OF LOWER DEGREE. THE LEADING ZERO-COEFFICIENTS ARE DISCARDED, AND THE ZEROS OF THE RESULTING POLYNOMIAL WILL BE CALCULATED. THE NUMBER OF LEADING ZERO-COEFFICIENTS WILL BE ADDED TO THE NUMBER OF NOT-FOUND EIGENVALUES OF THE COMPANION MATRIX, IN ORDER TO PRESERVE THE RELATIONSHIP: NOT-FOUND ZEROS + FOUND ZEROS = DEGREE OF POLYNOMIAL.
2. SUPPOSE Z IS THE NUMBER OF ZEROS EQUAL TO 0, THEN INSTEAD OF THE POLYNOMIAL GIVEN BY STEP 1, THIS POLYNOMIAL DIVIDED BY  $X^{**Z}$  WILL BE HANDLED. MOREOVER, Z ZERO'S WILL BE ADDED TO THE EIGENVALUES FOUND BY COMVALQRI.
3. LET NZ BE THE DEGREE OF THE POLYNOMIAL OBTAINED IN STEP 2, AND C(I) THE COEFFICIENT OF  $X^{**I}$ . A SQUARE ARRAY AA IS INITIALIZED BY SETTING:
 

AA[1,J] := - C[NZ-J] / C[NZ],	J = 1 ... NZ;
AA[J+1,J] := 1,	J = 1 ... NZ-1;
AA[I,J] := 0,	FOR ALL OTHER ELEMENTS.

 MOREOVER AN UPPERBOUND FOR THE ZEROS IS OBTAINED BY CALCULATING  $\text{MAX}(\text{ABS}(C[I]/C[NZ])^{**} (1/(NZ-I)))$ , AND THIS VALUE IS USED AS THE NORM OF THE MATRIX.
4. THE MATRIX SO OBTAINED IS EQUILIBRATED IN A WAY ANALOGOUS TO THE PROCEDURE EQUILBR (SECTION 3.2.1.1.1). HOWEVER, IF  $(\text{SUM}(A[I,J]^{**}2) \text{ OVER } J = \text{SUM}(A[J,I]^{**}2) \text{ OVER } J)$  FOR  $I > 1$  THIS EQUATION IMMEDIATELY HOLDS FOR  $I = 1$ , SO THERE IS NO NEED TO USE THE FIRST ROW AND COLUMN IN THIS PROCESS (AND INDEED THE FIRST ROW IS THE ONLY ROW CONTAINING MORE THAN 1 NON-ZERO ELEMENT). IN FACT, THIS EQUILIBRATING PROCESS IS PERFORMED ON TWO ONE-DIMENSIONAL ARRAYS.

AFTER THESE FOUR STEPS, THE PROCEDURE COMVALQRI IS CALLED, AND THE FOLLOWING STEPS ARE TAKEN:

1. THE ZEROS EQUAL TO 0 ARE ADDED AT THE END OF THE ARRAYS RE AND IM,
2. IF THE ORIGINAL POLYNOMIAL CONTAINED SOME LEADING ZERO-COEFFICIENTS, ALL ZEROS ARE SHIFTED TOWARDS THE END IN THE ARRAYS RE AND IM IN ORDER TO GUARANTEE THAT ALL ZEROS FOUND ARE STORED IN THE LAST PARTS OF THESE ARRAYS.

THE PROCEDURE COMVALQRI AND THE PROCESS GIVEN ABOVE GUARANTEE A GOOD PRECISION FOR WELL-SEPARATED ZEROS, AND (IF PRESENT) A MULTIPLE ZERO EQUAL TO 0. HOWEVER, IF THE POLYNOMIAL HAS NOT-WELL-SEPARATED ZEROS, A HIGH PRECISION CANNOT BE GUARANTEED. IN FACT A DOUBLE ZERO CANNOT BE GUARANTEED TO BE CORRECT IN MORE THAN HALF THE WORD-LENGTH, AS THE COMPANION MATRIX IS DEFECTIVE. IN THE EXAMPLE GIVEN BELOW, ONE FINDS INDEED ALL ZEROS CORRECT IN 12 DIGITS, WITH THE EXCEPTION OF THE DOUBLE ZERO 1, WHICH HAS BEEN CALCULATED WITH A SUBSTANTIAL IMAGINARY PART.

LANGUAGE: ALGOL-60.

EXAMPLE OF USE:

WE NEXT GIVE A PROGRAM FOLLOWED BY ITS OUTPUT:

```
"BEGIN" "INTEGER" I;
  "ARRAY" A[0:7], RE, IM[1:7], EM[0:5];

  "INTEGER" "PROCEDURE" POLZEROS(A, N, EM, RE, IM);
  "VALUE" N; "INTEGER" N; "ARRAY" A, EM, RE, IM;
  "CODE" 34500;

  A[1]:= - 12; A[2]:= 38; A[3]:= - 46; A[4]:= 25;
  A[5]:= - 3; A[6]:= - 3; A[7]:= 1; A[0]:= 0;
  EM[0]:= "-14; EM[2]:= "-13; EM[4]:= 60;
  I:= POLZEROS(A, 7, EM, RE, IM);
  OUTPUT(61, "("("NUMBER NOT FOUND ZEROS ")", 3ZD, /,
    "("UPPERBOUND OF THE ZEROS ")", N, /,
    "("MAXIMAL NEGLECTED SUBDIAGONAL ELEMENT ")", N, /,
    "("NUMBER OF ITERATIONS ")", 3ZD, /)"", I, EM[1], EM[3], EM[5]);
  OUTPUT(61, "("/, "("ZEROS :")", /)"");
  "FOR" I:= 1 "STEP" 1 "UNTIL" 7 "DO"
  "IF" IM[I] = 0 "THEN" OUTPUT(61, "("/, ZDSB, N)"", I, RE[I])
  "ELSE" OUTPUT(61, "("/, ZDSB, 2(N)"", I, RE[I], IM[I])
"END"
```

```
NUMBER NOT FOUND ZEROS      0
UPPERBOUND OF THE ZEROS +6.000000000000000"+000
MAXIMAL NEGLECTED SUBDIAGONAL ELEMENT +4.0203975643582"-015
NUMBER OF ITERATIONS      10
```

ZEROS :

1	-2.999999999999998"+000	
2	+2.000000000000000"+000	
3	+1.000000000000001"+000	+1.000000000000000"+000
4	+1.000000000000001"+000	-1.000000000000000"+000
5	+9.99999999999980"-001	+4.3687070347008"-007
6	+9.99999999999980"-001	-4.3687070347008"-007
7	+0.000000000000000"+000	

## SOURCE TEXT(S):

```

"CODE" 34500;
"INTEGER" "PROCEDURE" POLZEROS(A, N, EM, RE, IM);
"VALUE" N; "INTEGER" N; "ARRAY" A, EM, RE, IM;
"BEGIN" "INTEGER" INF, ZERO, I, J, NI, EXPONENT, NZ, NZI;
      "REAL" FACTOR, C, R, Z, NORM;

      "INTEGER" "PROCEDURE" COMVALGRI(A, N, EM, RE, IM);
      "VALUE" N; "INTEGER" N; "ARRAY" A, EM, RE, IM;
      "CODE" 34190;

INF:= 0;
"FOR" I:= N "WHILE" A[I] = 0 "AND" I > 0 "DO"
"BEGIN" INF:= INF + 1; NZ:= N - 1 "END";
ZERO:= 0; I:= - 1;
"FOR" I:= I + 1 "WHILE" A[I] = 0 "AND" I < N "DO"
"BEGIN" ZERO:= ZERO + 1; RE[N - I]:= IM[N - I]:= 0 "END";
NZ:= N - ZERO; "IF" NZ > 0 "THEN"
"BEGIN" "ARRAY" AA[1:NZ,1:NZ], B[1:NZ];
      "FOR" I:= 2 "STEP" 1 "UNTIL" NZ "DO"
      "BEGIN" "FOR" J:= 1 "STEP" 1 "UNTIL" NZ "DO" AA[I,J]:= 0;
        B[I - 1]:= 1
      "END";
      Z:= A[N]; NORM:= 0; B[NZ]:= 0; NI:= NZ; NZI:= 0;
      "FOR" I:= ZERO + 1 "STEP" 1 "UNTIL" N "DO"
      "BEGIN" A[NZI]:= R:= - A[I - 1] / Z; NZI:= NZI + 1;
        R:= ABS(R) ** (1 / NI); "IF" R > NORM "THEN" NORM:= R;
        NI:= NI - 1
      "END";
      EM[1]:= NORM * 2; FACTOR:= 1 / (2 * LN(2)); I:= 1; NI:= NZ - 1;
      "FOR" I:= "IF" I < NZ "THEN" I + 1 "ELSE" 2 "WHILE" NI > 0 "DO"
      "BEGIN" NZI:= NZ - I; C:= SQRT(A[NZI] ** 2 + B[I] ** 2);
        R:= ABS(B[I - 1]); EXPONENT:= LN(R / C) * FACTOR;
        "IF" ABS(EXPONENT) > 1 "THEN"
        "BEGIN" NI:= NZ - 1; C:= 2 ** EXPONENT; R:= 1 / C;
          B[I - 1]:= B[I - 1] * R; A[NZI]:= A[NZI] * C;
          B[I]:= B[I] * C
        "END"
        "ELSE" NI:= NI - 1
      "END";
      NZI:= NZ - 1;
      "FOR" I:= 1 "STEP" 1 "UNTIL" NZ "DO"
      "BEGIN" AA[1,I]:= A[NZI]; NZI:= NZI - 1;
        "IF" I < NZ "THEN" AA[I + 1,I]:= B[I]
      "END";
      POLZEROS:= COMVALGRI(AA, NZ, EM, RE, IM) + INF;
"END"
"ELSE" POLZEROS:= INF;
"IF" INF = 0 "THEN"
"FOR" I:= N "STEP" - 1 "UNTIL" 1 "DO"
"BEGIN" RE[I + INF]:= RE[I]; IM[I + INF]:= IM[I] "END"
"END" POLZEROS;
"EOP"

```



SECTION : 3.6.2

(NOVEMBER 1976)

PAGE 1

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RECEIVED: 740520.

BRIEF DESCRIPTION:

THIS SECTION CONTAINS FIVE PROCEDURES FOR CALCULATING ZEROS OF ORTHOGONAL POLYNOMIALS WHICH ARE GIVEN BY THE COEFFICIENTS OF THEIR RECURRENCE RELATION;  
ALLZERORTPOL CALCULATES ALL ZEROS,  
LUPZERORTPOL CALCULATES A NUMBER OF ADJACENT UPPER OR LOWER ZEROS,  
SELZERORTPOL CALCULATES A NUMBER OF ADJACENT ZEROS.  
IT IS EFFICIENT TO USE ALLZERORTPOL IF MORE THAN 50 PERCENT OF EXTREME ZEROS OR MORE THAN 25 PERCENT OF SELECTED ZEROS ARE WANTED.  
ALLJACZER CALCULATES THE ZEROS OF THE N-TH JACOBIAN POLYNOMIAL. 3  
ALLLAGZER CALCULATES THE ZEROS OF THE N-TH LAGUERRE POLYNOMIAL.

KEYWORDS:

ZEROS,  
ORTHOGONAL POLYNOMIALS,  
CHRISTOFFEL ABSCISSAS.

SUBSECTION: ALLZERORTPOL.

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "PROCEDURE" ALLZERORTPOL (N, B, C, ZER, EM);  
 "VALUE" N; "INTEGER" N; "ARRAY" B, C, ZER, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

B, C: <ARRAY IDENTIFIER>;  
 "ARRAY" B, C (0:N-1);  
 ENTRY: THE ELEMENTS B[I] AND C[I],  $I = 0, 1, \dots, N-1$ ,  
 CONTAIN THE COEFFICIENTS OF THE RECURRENCE RELATION  
 $P_{I+1}(X) = (X - B[I]) * P_I(X) - C[I] * P_{I-1}(X)$   
 $I = 0, 1, \dots, N-1$ ,  
 $C[0] = 0$ ;

ZER: <ARRAY IDENTIFIER>;  
 "ARRAY" ZER(1:N);  
 EXIT: THE ZEROS OF THE N-TH DEGREE ORTHOGONAL POLYNOMIAL;

N: <ARITHMETIC EXPRESSION>;  
 ENTRY: THE DEGREE OF THE ORTHOGONAL POLYNOMIAL OF WHICH  
 THE ZEROS ARE TO BE CALCULATED;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM(0:5);  
 ENTRY: EM[0]: THE MACHINE PRECISION;  
 EM[2]: THE RELATIVE TOLERANCE OF THE ZEROS;  
 EM[4]: THE MAXIMUM ALLOWED NUMBER OF ITERATIONS,  
 E.G.  $5 * N$ ;

EXIT: EM[1]: THE MAXIMUM OF  $ABS(B[0]) + 1$ ,  
 $C[I] + ABS(B[I]) + 1$ , ( $I=1, \dots, N-2$ ),  
 $C[N-1] + ABS(B[N-1])$ ;  
 EM[3]: INFORMATION CONCERNING THE PROCESS USED;  
 I.E. THE MAXIMUM ABSOLUTE VALUE OF THE  
 CODIAGONAL ELEMENTS NEGLECTED,  
 (SEE ALSO SECTION 3.3.1.1.1.);  
 EM[5]: THE NUMBER OF ITERATIONS PERFORMED.

SECTION : 3.6.2

(NOVEMBER 1976)

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## PROCEDURES USED:

GRIVALSYMTRI     = CP34160,  
 DUPVEC           = CP31030.

METHOD AND PERFORMANCE : SEE SELZERORTPOL (THIS SECTION).

REFERENCES : SEE ALL LAG ZER (THIS SECTION).

## EXAMPLE OF USE:

AS A FORMAL TEST OF THE PROCEDURE WE CALCULATE THE ZEROS OF THE CHEBYSHEV POLYNOMIAL (OF THE FIRST KIND) OF THE THIRD DEGREE. THE RECURRENCE COEFFICIENTS ARE:

$B[1] = 0, I = 0, 1, 2;$

$C[0] = 0, C[1] = .5, C[2] = .25.$

(IT IS RECOMMENDED TO STORE THE ELEMENTS OF THE ARRAYS B AND C IN REVERSED ORDER IF THESE ELEMENTS ARE STRONGLY INCREASING).

```
"BEGIN" "ARRAY" B, C(0:3), ZER(1:3), EM(0:5);
"PROCEDURE" ALLZERORTPOL(N,B,C,ZER,EM);"CODE"31362;
EM(0):= EM(2):= "-14"; EM(4):=15;
B(2):=B(1):=B(0):=0;
C(0):= 0; C(1):= .5; C(2):= .25;
ALLZERORTPOL (3, B, C, ZER, EM);
OUTPUT(61, "("("THE THREE ZEROS:"), /, 3(/ZDSB,N), 2/,
           "("EM(1):")", 5BD.2D"+2D, /,
           "("EM(3):")", 5BD.2D"+2D, /, "("EM(5):")", 5ZD)"",
           1, ZER(1), 2, ZER(2), 3, ZER(3), EM(1), EM(3), EM(5))
"END"
```

## THE THREE ZEROS:

```
1        =8.6602540378444"-001
2        +8.6602540378444"-001
3        +7.3562436480607"-016
```

```
EM(1):     1.50"+00
EM(3):     1.42"-34
EM(5):     5
```

SECTION : 3.6.2

(OCTOBER 1974)

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SUBSECTION: LUPZERORTPOL.

## CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "PROCEDURE" LUPZERORTPOL (N, M, B, C, ZER, EM);  
 "VALUE" N, M; "INTEGER" N, M; "ARRAY" B, C, ZER, EM;

THE MEANING OF THE FORMAL PARAMETERS IS:

B, C: <ARRAY IDENTIFIER>;  
 "ARRAY" B, C [0:N-1];  
 ENTRY: THE ELEMENTS B[I] AND C[I],  $I = 0, 1, \dots, N-1$ ,  
 CONTAIN THE COEFFICIENTS OF THE RECURRENCE RELATION  
 $P[I+1](X) = (X - B[I]) * P[I](X) - C[I] * P[I-1](X)$   
 $I = 0, 1, \dots, N-1$ ,  
 $C[0] = 0$ ;

ZER: <ARRAY IDENTIFIER>;  
 "ARRAY" ZER[1:M];  
 EXIT: THE M LOWEST ZEROS ARE DELIVERED;  
 IF HOWEVER THE ARRAY B[0:N-1] CONTAINED THE OPPOSIT  
 VALUES OF THE CORRESPONDING RECURRENCE COEFFICIENTS  
 THEN THE OPPOSITE VALUES OF THE M UPPER ZEROS  
 ARE DELIVERED.  
 IN EITHER CASE,  $ZER[I] < ZER[I+1]$ ,  $I = 1, \dots, M-1$ ;

N: <ARITHMETIC EXPRESSION>;  
 ENTRY: THE DEGREE OF THE ORTHOGONAL POLYNOMIAL OF WHICH  
 THE ZEROS ARE TO BE CALCULATED;

M: <ARITHMETIC EXPRESSION>;  
 ENTRY: THE NUMBER OF ZEROS TO BE CALCULATED;

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM[0:5];  
 ENTRY: EM[0]: THE MACHINE PRECISION,  
 EM[2]: THE RELATIVE TOLERANCE OF THE ZEROS;  
 EM[4]: THE MAXIMUM ALLOWED NUMBER OF ITERATIONS,  
 E.G.  $15 * M$ ;  
 EM[6]: IF ALL ZEROS ARE KNOWN TO BE POSITIVE  
 THEN 1 ELSE 0;

EXIT: EM[1]: THE MAXIMUM OF  $ABS(B[0]) + 1$ ,  
 $C[I] + ABS(B[I]) + 1$ , ( $I=1, \dots, N-2$ ),  
 $C[N-1] + ABS(B[N-1])$ ;  
 EM[3]: INFORMATION CONCERNING THE PROCESS USED;  
 I.E. THE MAXIMUM ABSOLUTE VALUE OF THE  
 THEORETICAL ERRORS OF THE ZEROS  
 (SEE WILKINSON AND REINSCH, 1971, P.263);  
 EM[5]: THE NUMBER OF ITERATIONS PERFORMED.

## PROCEDURES USED:

DUPVEC = CP31030.  
 ABSMAXVEC = CP31060.

METHOD AND PERFORMANCE : SEE SELZERORTPOL (THIS SECTION).

REFERENCES : SEE ALL LAG ZER (THIS SECTION).

EXAMPLE OF USE:

AS A FORMAL TEST OF THE PROCEDURE WE CALCULATE THE TWO LOWER AND THE TWO UPPER ZEROS OF THE LAGUERRE POLYNOMIAL OF THE THIRD DEGREE.

THE RECURRENCE COEFFICIENTS ARE OBTAINED FROM [1], P.782:

$$B[I] = -A2I / A3I = 2I + 1;$$

$$C[I] = A4I / (A3I * A3(I-1)) * A1(I-1) = I * I, I = 0, 1, 2.$$

(IT IS RECOMMENDED TO STORE THE ELEMENTS OF THE ARRAYS B AND C IN REVERSED ORDER IF THESE ELEMENTS ARE STRONGLY DECREASING).

```
"BEGIN" "ARRAY" B, C(0:3), ZER(1:2), EM(0:6);
"INTEGER" I;
"PROCEDURE" LUPZERORTPOL(N,M,B,C,ZER,EM); "CODE" 31363;
EM(0) := EM(2) := -14; EM(4) := 45; EM(6) := 1;
"FOR" I := 0, 1, 2 "DO"
"BEGIN" B[I] := 2 * I + 1; C[I] := I * I "END";
LUPZERORTPOL (3, 2, B, C, ZER, EM);
OUTPUT(61, "("("THE TWO LOWER ZEROS:")", /, 2(/ZD5B,N), 2/,
"("EM[1]:")", 5BD.2D"+2D, /,
"("EM[3]:")", 5BD.2D"+2D, /, "("EM[5]:")", 5ZD")",
1, ZER[1], 2, ZER[2], EM[1], EM[3], EM[5]);
EM(6) := 0;
"FOR" I := 0, 1, 2 "DO"
"BEGIN" B[I] := -2 * I - 1; C[I] := I * I "END";
LUPZERORTPOL (3, 2, B, C, ZER, EM);
OUTPUT(61, "("3/, "("("THE TWO UPPER ZEROS:")", /, 2(/ZD5B,N), 2/,
"("EM[1]:")", 5BD.2D"+2D, /,
"("EM[3]:")", 5BD.2D"+2D, /, "("EM[5]:")", 5ZD")",
1, -ZER[1], 2, -ZER[2], EM[1], EM[3], EM[5]);
"END"
```

THE TWO LOWER ZEROS:

```
1      +4.1577455678348"-001
2      +2.2942803602791"+000
```

```
EM[1]:      9.00"+00
EM[3]:      5.72"-16
EM[5]:      12
```

THE TWO UPPER ZEROS:

```
1      +6.2899450829375"+000
2      +2.2942803602791"+000
```

```
EM[1]:      9.00"+00
EM[3]:      4.70"-20
EM[5]:      14
```

SUBSECTION: SELZERORTPOL.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "PROCEDURE" SELZERORTPOL (N, N1, N2, B, C, ZER, EM);  
 "VALUE" N, N1, N2; "INTEGER" N, N1, N2; "ARRAY" B, C, ZER, EM;

THE MEANING OF THE FORMAL PARAMETERS IS :

B, C: <ARRAY IDENTIFIER>;  
 "ARRAY" B, C [0 : N-1];  
 ENTRY: THE ELEMENTS B[I] AND C[I],  $I = 0, 1, \dots, N-1$ ,  
 CONTAIN THE COEFFICIENTS OF THE RECURRENCE RELATION  
 $P[I+1](X) = (X - B[I]) * P[I](X) - C[I] * P[I-1](X)$   
 $I = 0, 1, \dots, N-1$ ,  
 $C[0] = 0$ ;

ZER: <ARRAY IDENTIFIER>;  
 "ARRAY" ZER [N1:N2];  
 EXIT: THE  $N2-N1+1$  CALCULATED ZEROS IN DECREASING ORDER.

N, N1, N2: <ARITHMETIC EXPRESSION>;  
 ENTRY: N IS THE DEGREE OF THE ORTHOGONAL POLYNOMIAL OF  
 WHICH THE  $N1$ -TH UP TO AND INCLUDING  $N2$ -TH ZEROS ARE  
 TO BE CALCULATED ( $ZER[N1] \geq ZER[N2]$ );

EM: <ARRAY IDENTIFIER>;  
 "ARRAY" EM [0:5];  
 ENTRY: EM[0]: THE MACHINE PRECISION.  
 EM[2]: THE RELATIVE TOLERANCE OF THE ZEROS;  
 EXIT: EM[1]: THE MAXIMUM OF  $ABS(B[0]) + 1$ ,  
 $C[I] + ABS(B[I]) + 1$  ( $I=1, \dots, N-2$ ) AND  
 $C[N-1] + ABS(B[N-1])$ ;  
 EM[5]: THE NUMBER OF ITERATIONS PERFORMED.

PROCEDURES USED:

VALSYMTRI = CP34151.

METHOD AND PERFORMANCE:

THE ZEROS OF AN ORTHOGONAL POLYNOMIAL ARE THE EIGENVALUES OF A  
 SYMMETRIC TRIDIAGONAL MATRIX (SEE [2], [3], P. 375, 376, [4], P. 120).  
 THE ORTHOGONAL POLYNOMIAL IS DEFINED BY A LINEAR THREE-TERM  
 HOMOGENEOUS RECURRENCE RELATION.

REFERENCES : SEE ALL LAG ZER (THIS SECTION).

## EXAMPLE OF USE :

AS A FORMAL TEST OF THE PROCEDURE WE CALCULATE THE THIRD ZERO OF THE LEGENDRE POLYNOMIAL OF THE FOURTH DEGREE.

THE RECURRENCE COEFFICIENTS ARE OBTAINED FROM [1], P.782:

$B[I] = 0, I = 0, 1, 2, 3;$

$C[I] = A4I / (A3I + A3(I-1)) * A1(I-1) = I * I / (4 * I * I - 1),$   
 $I = 0, 1, 2, 3.$

(IT IS RECOMMENDED TO STORE THE ELEMENTS OF THE ARRAYS B AND C IN REVERSED ORDER IF THESE ELEMENTS ARE STRONGLY DECREASING).

```
"BEGIN" "ARRAY" B, C[0:4], ZER[3:3], EM[0:5];
"INTEGER" I;
"PROCEDURE" SELZERORTPOL (N,N1,N2,B,C,ZER,EM);"CODE"31364;
EM[0]:= EM[2] := "-14;
"FOR" I:= 0, 1, 2, 3 "DO"
"BEGIN" B[I]:= 0; C[I]:= I * I / (4 * I * I - 1) "END";
SELZERORTPOL (4, 3, 3, B, C, ZER, EM);
OUTPUT(61, "("("THE THIRD ZERO:"),2/,ZDSB,N,2/,
          "("EM[1]:)",5BD,2D"+2D, /,
          "("EM[5]:)",5ZD")",3,ZER[3],EM[1],EM[5])
"END"
```

THE THIRD ZERO:

3        =3.3998104358486"-001

EM[1]:        1.33"+00

EM[5]:        12

SUBSECTION: ALL JAC ZER.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:

```
"PROCEDURE" ALL JAC ZER(N, ALFA, BETA, ZER);
"VALUE" N, ALFA, BETA;
"INTEGER" N; "REAL" ALFA, BETA; "ARRAY" ZER;
"CODE" 31370;
```

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;

THE UPPER BOUND OF THE ARRAY ZER;  $N \geq 1$ ;

ALFA, BETA: <ARITHMETIC EXPRESSION>;

THE PARAMETERS OF THE JACOBI POLYNOMIAL, SEE [1];

ALFA, BETA  $> = 1$ ;

ZER: <ARRAY IDENTIFIER>;

"ARRAY" ZER[1 : N];

EXIT: ZER[1], ..., ZER[N] ARE THE ZEROS OF THE N-TH JACOBI POLYNOMIAL WITH PARAMETERS ALFA AND BETA.

## PROCEDURES USED:

ALL ZER ORT POL = CP 31362.

## REQUIRED CENTRAL MEMORY:

IF ALFA = BETA THE TWO AUXILIARY ARRAYS OF N//2 REALS ARE USED, OTHERWISE TWO AUXILIARY ARRAYS OF N REALS ARE DECLARED.

## METHOD AND PERFORMANCE:

THE JACOBI POLYNOMIALS ARE A SPECIAL CASE OF ORTHOGONAL POLYNOMIALS (SEE [1]); ALL JAC ZER COMPUTES THE COEFFICIENTS OF THE THREE-TERM RECURRENCE RELATION AND CALLS THE PROCEDURE ALL ZER ORT POL TO COMPUTE THE ZEROS; IF ALFA = BETA, THE POLYNOMIALS ARE ODD OR EVEN, HENCE ONLY THE THE POSITIVE ZEROS ARE CALCULATED; THIS IS DONE BY MEANS OF THE FORMULAS

$$P(2*M, ALFA, ALFA, X) = C(M)*P(M, ALFA, -0.5, 2*X*X - 1),$$

$$P(2*M - 1, ALFA, ALFA, X) = D(M)*P(M, ALFA, +0.5, 2*X*X - 1)*X$$

(SEE [1], FORMULAS 22.5.20 - 22.5.27).

## EXAMPLE OF USE:

THE PROGRAM

```
"BEGIN" "ARRAY" X[1:3];
  "PROCEDURE" ALL JAC ZER(N, ALFA, BETA, ZER); "CODE" 31370;
  ALL JAC ZER(3, .5, .5, X);
  OUTPUT(61, ("3(4B=D.13D)=ZD"), X[1], X[2], X[3])
"END"
```

PRINTS THE FOLOWING RESULTS:

•8.6602540378444"-1      0.00000000000000" 0      8.6602540378444"-1

REFERENCES : SEE ALL LAG ZER(THIS SECTION).



SUBSECTION: ALL LAG ZER.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:

"PROCEDURE" ALL LAG ZER(N, ALFA, ZER);  
"VALUE" N, ALFA;  
"INTEGER" N; "REAL" ALFA; "ARRAY" ZER;  
"CODE" 31371;

THE MEANING OF THE FORMAL PARAMETERS IS:

N: <ARITHMETIC EXPRESSION>;  
THE UPPER BOUND OF THE ARRAY ZER;  $N \geq 1$ ;  
ALFA: <ARITHMETIC EXPRESSION>;  
THE PARAMETER OF THE LAGUERRE POLYNOMIAL, SEE [1];  $ALFA > -1$ ;  
ZER: <ARRAY IDENTIFIER>;  
"ARRAY" ZER(1 : N);  
EXIT: ZER(1), ..., ZER(N) ARE THE ZEROS OF THE N-TH  
LAGUERRE POLYNOMIAL WITH PARAMETER ALFA.

PROCEDURES USED:

ALL ZER ORT POL = CP 31362.

REQUIRED CENTRAL MEMORY:

TWO AUXILIARY ARRAYS OF N REALS ARE USED.

METHOD AND PERFORMANCE:

THE LAGUERRE POLYNOMIALS ARE A SPECIAL CASE OF ORTHOGONAL  
POLYNOMIALS (SEE [1]); ALL LAG ZER COMPUTES THE COEFFICIENTS  
OF THE THREE-TERM RECURRENCE RELATION AND CALLS THE PROCEDURE  
ALL ZER ORT POL TO COMPUTE THE ZEROS.

REFERENCES :

- [1] : M. ABRAMOWITZ AND I.A. STEGUN(1965):  
HANDBOOK OF MATHEMATICAL FUNCTIONS.  
DOVER PUBLICATIONS INC.
- [2] : G.H. GOLUB AND J.H. WELSCH(1969):  
CALCULATION OF GAUSS QUADRATURE RULES.  
MATH. COMP. VOL. 23,P.221-230.
- [3] : C. LANCZOS(1957):  
APPLIED ANALYSIS.  
PRENTICE HALL.
- [4] : J. STOER(1972):  
EINFUEHRUNG IN DIE NUMERISCHE MATHEMATIK 1.  
HEIDELBERGER TASCHENBUECHER 105,SPRINGER.

EXAMPLE OF USE:

THE PROGRAM

```
"BEGIN" "ARRAY" X[1:3];  
  "PROCEDURE" ALL LAG ZER(N, ALFA, ZER); "CODE" 31371;  
  ALL LAG ZER(3,=.5,X);  
  OUTPUT(61, ("3(4B=D.13D"-ZD)"), X[1], X[2], X[3])  
"END"
```

PRINTS THE FOLOWING RESULTS:

1.9016350919350" =1      1.7844927485432" 0      5.5253437422633" 0.

## SOURCE TEXT(S) :

```

"CODE"31362;
"PROCEDURE" ALLZERORTPOL (N, B, C, ZER, EM);
"VALUE" N; "INTEGER" N; "ARRAY" B, C, ZER, EM;
"BEGIN" "INTEGER" I; "REAL" NRM;
  "INTEGER" "PROCEDURE" QRIVALSYMTRI (D, BB, N, EM); "CODE" 34160;
  "PROCEDURE" DUPVEC (L, U, SHIFT, A, B); "CODE" 31030;
  C[N] := 0;
  NRM := ABS(B[0]);
  "FOR" I := 1 "STEP" 1 "UNTIL" N-2 "DO" "IF" C[I] + ABS(B[I]) > NRM "THEN"
    NRM := C[I] + ABS(B[I]);
    "IF" N > 1 "THEN" NRM := "IF" NRM + 1 > C[N-1] + ABS(B[N-1]) "THEN" NRM + 1 "ELSE"
      C[N-1] + ABS(B[N-1]);
  EM[1] := NRM;
  "FOR" I := N "STEP" -1 "UNTIL" 1 "DO" B[I] := B[I - 1];
  QRIVALSYMTRI (B, C, N, EM);
  DUPVEC (1, N, 0, ZER, B)
"END" ALLZERORTPOL;
  "EOP"

"CODE"31363;
"PROCEDURE" LUPZERORTPOL (N, M, B, C, ZER, EM);
"VALUE" N, M; "INTEGER" N, M; "ARRAY" B, C, ZER, EM;
"BEGIN"
"PROCEDURE" RATQR(N,M,POSDEF,DLAM,EPS)TRANS;(D,B2);
  "VALUE" N,M,POSDEF,DLAM,EPS;
  "INTEGER" N,M;
  "BOOLEAN" POSDEF;
  "REAL" DLAM,EPS;
  "ARRAY" D,B2;
"COMMENT" QR ALGORITHM FOR THE COMPUTATION OF THE LOWEST EIGENVALUES
OF A SYMMETRIC TRIDIAGONAL MATRIX. A RATIONAL VARIANT OF THE
QR TRANSFORMATION IS USED, CONSISTING OF TWO SUCCESSIVE QR STEPS
PER ITERATION.
A SHIFT OF THE SPECTRUM AFTER EACH ITERATION GIVES AN ACCELERATED
RATE OF CONVERGENCE. A NEWTON CORRECTION, DERIVED FROM THE
CHARACTERISTIC POLYNOMIAL, IS USED AS SHIFT.
RATQR IS IMPLEMENTED BY REINSCH AND BAUER, SEE WILKINSON AND REINSCH
,1971, CONTR. II-6. (IN FUTURE RATQR MUST BE REPLACED BY RATQRI
(=CP34166)).
  FORHATS: D,B2[1:N];
"COMMENT"

```

```

"BEGIN"
  "INTEGER" I,J,K,T; "REAL" DELTA,E,EP,ERR,P,Q,QP,R,S,TOT;
  "REAL" "PROCEDURE" ABSMAXVEC(K,LOW,UP,A); "CODE" 31060;
  "COMMENT" LOWER BOUND FOR EIGENVALUES FROM GERSHGORIN, INITIAL SHIFT;
  B2[I] := ERR; Q := S := 0; TOT := D[I];
  "FOR" I := N "STEP" -1 "UNTIL" 1 "DO"
    "BEGIN"
      P := Q; Q := SQRT(B2[I]); E := D[I] - P - Q;
      "IF" E < TOT "THEN" TOT := E
    "END" I;
  "IF" POSDEF & TOT < 0 "THEN" TOT := 0 "ELSE"
  "FOR" I := 1 "STEP" 1 "UNTIL" N "DO" D[I] := D[I] - TOT;
  T := 0;
  "FOR" K := 1 "STEP" 1 "UNTIL" M "DO"
    "BEGIN"
  NEXT QR TRANSFORMATION; T := T + 1;
  TOT := TOT + S; DELTA := D[N] - S; I := N;
  E := ABS(EP * TOT); "IF" DLAM < E "THEN" DLAM := E;
  "IF" DELTA < = DLAM "THEN" "GOTO" CONVERGENCE;
  E := B2[N] / DELTA; QP := DELTA + E; P := 1;
  "FOR" I := N - 1 "STEP" -1 "UNTIL" K "DO"
    "BEGIN"
      Q := D[I] - S - E; R := Q / QP; P := P * R + 1;
      EP := E * R; D[I+1] := QP + EP; DELTA := Q - EP;
      "IF" DELTA < = DLAM "THEN" "GOTO" CONVERGENCE;
      E := B2[I] / Q; QP := DELTA + E; B2[I+1] := QP * EP
    "END" I;
  D[K] := QP; S := QP / P;
  "IF" TOT + S > TOT "THEN" "GOTO" NEXT QR TRANSFORMATION;
  "COMMENT" IRREGULAR END OF ITERATION,
  DEFLATE MINIMUM DIAGONAL ELEMENT;
  S := 0; I := K; DELTA := QP;
  "FOR" J := K + 1 "STEP" 1 "UNTIL" N "DO"
    "IF" D[J] < DELTA "THEN"
      "BEGIN" I := J; DELTA := D[J] "END";

```

"COMMENT"

CONVERGENCE;

```

"IF" I < N "THEN" B2[I+1] := B2[I]*E/OP;
"FOR" J := I-1 "STEP" -1 "UNTIL" K "DO"
  "BEGIN" D[J+1] := D[J]-S; B2[J+1] := B2[J] "END" J;
D[K] := TOT; B2[K] := ERR := ERR+ABS(DELTA)
"END" K;
EM[5] := T; EM[3] := ABSMAXVEC(T, 1, M, B2);
"END" RATQR;

```

```

"PROCEDURE" DUPVEC (L, U, SHIFT, A, B); "CODE" 31030;
"INTEGER" I; "REAL" NRM;
NRM := ABS(B[0]);
"FOR" I := 1 "STEP" 1 "UNTIL" N-2 "DO" "IF" C[I]+ABS(B[I]) > NRM "THEN"
  NRM := C[I]+ABS(B[I]);
  "IF" N > 1 "THEN" NRM := "IF" NRM+1 > C[N-1]+ABS(B[N-1]) "THEN" NRM+1 "ELSE"
    C[N-1]+ABS(B[N-1]);
EM[1] := NRM;
"FOR" I := N "STEP" -1 "UNTIL" 1 "DO"
  "BEGIN" B[I] := B[I-1]; C[I] := C[I-1] "END";
RATQR (N, M, EM[6] := 1, EM[2], EM[0], B, C);
DUPVEC (1, M, 0, ZER, B)
"END" LUPZERORTPOL;
"EOP"

```

```

"CODE" 31364;
"PROCEDURE" SELZERORTPOL (N, N1, N2, B, C, ZER, EM);
"VALUE" N, N1, N2; "INTEGER" N, N1, N2; "ARRAY" B, C, ZER, EM;
"BEGIN" "INTEGER" I; "REAL" NRM;
"PROCEDURE" VALSYMTRI (D, BB, N, N1, N2, VAL, EM); "CODE" 34151;
NRM := ABS(B[0]);
"FOR" I := N-2 "STEP" -1 "UNTIL" 1 "DO" "IF" C[I]+ABS(B[I]) > NRM "THEN"
  NRM := C[I]+ABS(B[I]);
  "IF" N > 1 "THEN" NRM := "IF" NRM+1 > C[N-1]+ABS(B[N-1]) "THEN" NRM+1 "ELSE"
    C[N-1]+ABS(B[N-1]);
EM[1] := NRM;
"FOR" I := N "STEP" -1 "UNTIL" 1 "DO" B[I] := B[I-1];
VALSYMTRI (B, C, N, N1, N2, ZER, EM);
EM[5] := EM[3];
"END" SELZERORTPOL;
"EOP"

```

```

"CODE" 31370;
"PROCEDURE" ALL JAC ZER(N, ALFA, BETA, ZER);
"VALUE" N, ALFA, BETA; "INTEGER" N;
"REAL" ALFA, BETA; "ARRAY" ZER;
"IF" ALFA = BETA "THEN"
"BEGIN" "INTEGER" I, M;
  "ARRAY" A, B[0:N//2], EM[0:5];
  "REAL" MIN, GAMMA, SUM, ZER;
  "PROCEDURE" ALL ZER ORT POL(N, A, B, ZER, EM); "CODE" 31362;
  "COMMENT"

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## SECTION 3.6.2

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M:= N//2; "IF" N # 2*M "THEN"
"BEGIN" GAMMA:= + 0.5; ZER[M + 1]:= 0 "END"
"ELSE" GAMMA:= - 0.5;
MIN:= 0.25 = ALFA*ALFA; SUM:= ALFA + GAMMA + 2;
A[0]:= (GAMMA - ALFA)/SUM; A[1]:= MIN/SUM/(SUM + 2);
B[1]:= 4*(1 + ALFA)*(1 + GAMMA)/SUM/SUM/(SUM + 1);
"FOR" I:= 2 "STEP" 1 "UNTIL" M = 1 "DO"
"BEGIN" SUM:= I + I + ALFA + GAMMA;
      A[I]:= MIN/SUM/(SUM + 2); SUM := SUM*SUM;
      B[I]:= 4*I*(I + ALFA + GAMMA)*(I + ALFA)*(I + GAMMA)/
      SUM/(SUM = 1)
"END";
EM[0]:= 7.2" = 15; EM[2]:= "-10; EM[4]:= 6*M;
ALL ZER ORT POL (M, A, B, ZER, EM);
"FOR" I:= 1 "STEP" 1 "UNTIL" M "DO"
"BEGIN" ZER[I]:= ZER[I] = SQR((1 + ZER[I])/2);
      ZER[N + 1 - I]:= - ZER[I]
"END"
"END" "ELSE"
"BEGIN" "INTEGER" I; "REAL" SUM, MIN;
"ARRAY" A, B[0:N], EM[0:5];
"PROCEDURE" ALL ZER ORT POL(N, A, B, ZER, EM); "CODE" 31362;
MIN:= (BETA - ALFA)*(BETA + ALFA);
SUM:= ALFA + BETA + 2; B[0]:= 0;
A[0]:= (BETA - ALFA)/SUM;
A[1]:= MIN/SUM/(SUM + 2);
B[1]:= 4*(1 + ALFA)*(1 + BETA)/SUM/SUM/(SUM + 1);
"FOR" I:= 2 "STEP" 1 "UNTIL" N = 1 "DO"
"BEGIN" SUM:= I + I + ALFA + BETA;
      A[I]:= MIN/SUM/(SUM + 2); SUM:= SUM*SUM;
      B[I]:= 4*I*(I + ALFA + BETA)*(I + ALFA)*(I + BETA)/
      (SUM = 1)/SUM
"END";
EM[0]:= 7.2" = 15; EM[2]:= 1.0"=8; EM[4]:= 6*N;
ALL ZER ORT POL(N, A, B, ZER, EM)
"END" ALL JAC ZER;
"EOB"

"CODE" 31371;
"PROCEDURE" ALL LAG ZER(N, ALFA, ZER);
"VALUE" N, ALFA ; "INTEGER" N; "REAL" ALFA ; "ARRAY" ZER;
"BEGIN" "INTEGER" I; "ARRAY" A, B[0:N], EM[0:5];
"PROCEDURE" ALL ZER ORT POL(N, A, B, ZER, EM); "CODE" 31362;
B[0]:= 0; A[N - 1]:= N + N + ALFA = 1;
"FOR" I:= 1 "STEP" 1 "UNTIL" N = 1 "DO"
"BEGIN" A[I - 1]:= I + I + ALFA = 1;
      B[I]:= I*(I + ALFA)
"END";
EM[0]:= 7.2" = 15; EM[2]:= "-10; EM[4]:= 6*N;
ALL ZER ORT POL(N, A, B, ZER, EM)
"END" ALL LAG ZER;
"EOB"

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SECTION : 3.6.3

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BRIEF DESCRIPTION:

COMKWD CALCULATES THE ROOTS OF A QUADRATIC EQUATION WITH COMPLEX COEFFICIENTS.

KEYWORDS:

ZEROS, QUADRATIC EQUATION, POLYNOMIAL EQUATION, COMPLEX COEFFICIENTS.

CALLING SEQUENCE:

THE HEADING OF THE PROCEDURE READS:  
 "PROCEDURE"COMKWD(PR,PI,QR,QI,GR,GI,KR,KI);  
 "VALUE"PR,PI,QR,QI;"REAL"PR,PI,QR,QI,GR,GI,KR,KI;

THE MEANING OF THE FORMAL PARAMETERS IS:  
 PR,PI,QR,QI:<ARITHMETIC EXPRESSION>;  
 ENTRY:PR,QR ARE THE REAL PARTS AND PI,QI ARE THE  
 IMAGINARY PARTS OF THE COEFFICIENTS OF THE  
 QUADRATIC EQUATION:  
 $X^2 + 2*(PR + I*PI)*X + (QR + I*QI) = 0;$   
 GR,GI,KR,KI:<VARIABLE>;  
 EXIT:THE REAL PARTS AND THE IMAGINARY PARTS OF THE  
 BINOMIAL ARE DELIVERED IN GR,KR AND GI,KI,  
 RESPECTIVELY;MOREOVER,THE MODULUS OF GR+I\*GI IS  
 GREATER OR EQUAL THE MODULUS OF KR+I\*KI.

PROCEDURES USED:

COMMUL=CP34341;  
 COMDIV=CP34342;  
 COMSQRT=CP34343.

LANGUAGE: ALGOL 60.

EXAMPLE OF USE:

```
"BEGIN" "REAL" GR, GI, KR, KI;
"PROCEDURE" COMKWD (PR, PI, QR, QI, GR, GI, KR, KI);
"CODE" 34345;
COMKWD (.1, .3, .11, .02, GR, GI, KR, KI);
OUTPUT (61, "(" ("X**2=2(-.1+.3*I)*X=(.11+.02*I) HAS ROOTS")", /,
        =D, DD, +D, DD, ("*I")", /,
        =D, DD, +D, DD, ("*I")""), GR, GI, KR, KI)
"END"
```

```
X**2=2(-.1+.3*I)*X=(.11+.02*I) HAS ROOTS
=0,30+0,40*I
 0,10+0,20*I
```

SOURCE TEXT(S):

```
"CODE" 34345;
"PROCEDURE" COMKWD (PR, PI, QR, QI, GR, GI, KR, KI);
"VALUE" PR, PI, QR, QI, "REAL" PR, PI, QR, QI, GR, GI, KR, KI;
"BEGIN"
"PROCEDURE" COMMUL (AR, AI, BR, BI, RR, RI);
"CODE" 34341;
"PROCEDURE" COMDIV (XR, XI, YR, YI, ZR, ZI);
"CODE" 34342;
"PROCEDURE" COMSQRT (AR, AI, PR, PI);
"CODE" 34343;
"IF" QR=0 & QI = 0 "THEN"
"BEGIN" KR:=KI:=0 ;GR:=PR*2;GI:=PI*2 "END" "ELSE"
"IF" PR=0 & PI= 0 "THEN"
"BEGIN" COMSQRT(QR, QI, GR, GI);KR:=GR;KI:=GI "END" "ELSE"
"BEGIN" "REAL" HR, HI;
"IF" ABS(PR) > 1 "OR" ABS(PI) >1 "THEN" "BEGIN"
COMDIV(QR, QI, PR, PI, HR, HI);
COMDIV(HR, HI, PR, PI, HR, HI);
COMSQRT(1+HR, HI, HR, HI);
COMMUL (PR, PI, HR+1, HI, GR, GI);
"END" "ELSE" "BEGIN" COMSQRT(QR+(PR+PI)*(PR=PI), QI+ PR*PI*2, HR, HI);
"IF" PR * HR + PI * HI > 0 "THEN"
"BEGIN" GR := PR + HR;GI := PI + HI "END" "ELSE"
"BEGIN" GR := PR - HR;GI:= PI - HI "END";
"END";
COMDIV(-QR, -QI, GR, GI, KR, KI);
"END"
"END" COMKWD;
"EQP"
```