

ALGORITHM 43

CROUT WITH PIVOTING II

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real procedure INNERPRODUCT (u,v) index : (k) start : (s)
finish : (f);

value s, f; **integer** k, s, f; **real** u, v;

comment INNERPRODUCT forms the sum of $u(k) \times v(k)$ for $k = s, s+1, \dots, f$. If $s > f$, the value of INNERPRODUCT is zero. The substitution of a very accurate inner product procedure would make CROUT more accurate;

comment INNERPRODUCT may be declared in the head of any block which includes the block in which CROUT is declared. It may be used independently for forming the inner product of vectors;

begin

real h;

h := 0; **for** k := s **step** 1 **until** f **do** **h** := h + u $\times$ v;

INNERPRODUCT := h

end INNERPRODUCT;

procedure CROUT II (A, b, n, y, pivot, det, repeat)

comment This procedure is a revision of Algorithm 16, Crout With Pivoting by George E. Forsythe, *Comm. ACM* 3, (1960) 507-8. In addition to modifications to improve the running of the program, and to conform to proper usage, it provides for the computation of the determinant, det, of the matrix A. The solution is obtained by Crout's method with row interchanges, as formulated in reference [1], for solving $Ay = b$ and transforming the augmented matrix $[A \ b]$ into its triangular decomposition LU with all $L(k,k) = 1$. If A is singular we exit to 'singular,' a nonlocal label. pivot (k) becomes the current row index of the pivot element in the k-th column. Thus enough information is preserved for the procedure to process a new right-hand side without repeating the triangularization, if the boolean parameter repeat is true. The accuracy obtainable from CROUT would be much increased by calling CROUT with a more accurate inner product procedure than INNERPRODUCT.

The contributions of Michael F. Lipp and George E. Forsythe by prepublication review and pointing out several errors are gratefully acknowledged;

comment Nonlocal identifiers appearing in this procedure are: (1) The nonlocal label 'singular', to which the procedure exits if $\det A = 0$, and (2) the real procedure 'INNERPRODUCT' given above;

value n; **array** A, b, y; **integer** n; **integer array** pivot; **real** det; **Boolean** repeat;

begin

integer k, i, j, imax, p; **real** TEMP, quot;

det := 1; **if** repeat **then go to** 6;

for k := 1 **step** 1 **until** n **do**

1: **begin**

TEMP := 0;

for i := k **step** 1 **until** n **do**

2: **begin**

A[i,k] := A[i,k] - INNERPRODUCT (A[i,p], A[p,k],
p, 1, k-1);

if abs(A[i,k]) > TEMP **then**

3: **begin**

TEMP := abs(A[i, k]); imax := i

end 3

end 2;

pivot [k] := imax;

comment We have found that A[imax, k] is the largest pivot in column k. Now we interchange rows k and imax;

if imax $\neq$ k **then**

4: **begin** det := - det; **for** j := 1 **step** 1 **until** n **do**

5: **begin**

TEMP := A[k,j]; A[k,j] := A[imax, j]; A[imax, j]
:= TEMP

end 5;

TEMP := b[k]; b[k] := b[imax]; b[imax] := TEMP

end 4;

comment The row interchange is done. We proceed to the elimination;

if A[k,k] = 0 **then go to** singular;

quot := 1.0/A[k,k];

for i := k+1 **step** 1 **until** n **do**

A[i,k] := quot $\times$ A[i,k];

for j := k+1 **step** 1 **until** n **do**

A[k,j] := A[k,j] - INNERPRODUCT (A[k,p]
A[p,j], p, 1, k-1);

b[k] := b[k] - INNERPRODUCT (A[k,p], b[p]
p, 1, k-1)

end 1; **go to** 7;

comment The triangular decomposition is now finished, and we skip to the back substitution;

6: **begin comment** This section is used when the formal parameter repeat is **true**, indicating that the matrix A has previously been decomposed into triangular form by CROUT II, with row interchanges specified by pivot, and that it is desired to solve the linear system with a new vector b, without repeating the triangularization;

for k := 1 **step** 1 **until** n **do**

begin

TEMP := b[pivot[k]]; b[pivot[k]] := b[k]; b[k] :=
TEMP; b[k] := b[k] - INNERPRODUCT
(A[k, p], b[p], p, 1, k-1) **end**;

end 6;

7: **for** k := n **step** - 1 **until** 1 **do**

8: **begin if** $\neg$ repeat **then** det := A[k,k] $\times$ det;

y[k] := (b[k] - INNERPRODUCT (A[k,p], y[p], p,
k+1, n)/A[k,k]

end 8;

end CROUT II;

REFERENCE:

- (1) J. H. WILKINSON, Theory and practice in linear systems. In John W. Carr III (editor), Application of Advanced Numerical Analysis to Digital Computers, pp. 43-100 (Lectures given at the University of Michigan, Summer 1958, College of Engineering, Engineering Summer Conferences, Ann Arbor, Michigan [1959]).

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CERTIFICATION OF ALGORITHM 43

CROUT II (Henry C. Thacher, Jr., *Comm. ACM*, 1960)

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CROUT II was coded by hand for the Royal Precision LGP-30 computer, using a 28-bit mantissa floating point interpretive system (24.2 modified).

The program was tested against the linear system:

$$A = \begin{pmatrix} 12.1719 & 27.3941 & 1.9827 & 7.3757 \\ 8.1163 & 23.3385 & 9.8397 & 4.9474 \\ 3.0706 & 13.5434 & 15.5973 & 7.5172 \\ 3.0581 & 3.1510 & 6.9841 & 13.1984 \end{pmatrix} \quad b = \begin{pmatrix} 6.6355 \\ 6.1304 \\ 4.6921 \\ 2.5393 \end{pmatrix}$$

with the following results:

$$A' = \begin{pmatrix} 12.171900 & 27.394100 & 1.9827000 & 7.3756999 \\ 0.25226957 & 6.6327021 & 15.097125 & 5.6565352 \\ 0.25124262 & -0.56260107 & 14.979620 & 14.527683 \\ 0.66680633 & 0.76468695 & -0.20207132 & -1.3606142 \end{pmatrix}$$

$$b' = \begin{pmatrix} 6.6354999 \\ 3.0181653 \\ 2.5702026 \\ -0.082780734 \end{pmatrix} \quad \text{pivot} = \begin{pmatrix} 1 \\ 3 \\ 4 \\ 4 \end{pmatrix} \quad y = \begin{pmatrix} 0.15929120 \\ 0.14691771 \\ 0.11257482 \\ 0.060840712 \end{pmatrix}$$

$\det = -1645.4499$. All elements of $Ab - y$ were less than 10^{-7} in magnitude. Identical results were obtained with the same b , and repeat **true**. With the same b and the last row vector of A replaced by $(19.1927, 33.4409, 25.1298, 5.2811)$, i.e. $A_{4,j} = A_{1,j} + 2A_{2,j} - 3A_{3,j}$, the results were:

$$\det = 0.10924352 \times 10^{-3},$$

$$y = (0.29214425 \times 10^8, -0.12131172 \times 10^8, 0.72411923 \times 10^7, -0.51018392 \times 10^7)$$

Failure to recognize this singular matrix is due to roundoff, either in the data input or in the calculation.

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The statement:

$$b[k] := g[k] - \text{INNERPRODUCT}(A[k,p], b[p], p, i, k-1)$$

should be:

$$b[k] := b[k] - \text{INNERPRODUCT}(A[k,p], b[p], 1, k-1)$$

The statement:

$$y[k] := (b[k] - \text{INNERPRODUCT}(A[k,p], y[p], p, k+1, n)) / A[k,k]$$

should be:

$$y[k] := (b[k] - \text{INNERPRODUCT}(A[k,p], y[p], p, k+1, n)) / A[k,k]$$

Storage may be saved eliminating the array y and using instead the array b , in which the solution is formed.

A previous certification of this algorithm [*Comm. ACM* 4, 4 (Apr. 1961), 182] was tested again with the same results. Two errors were detected in the certification: The row that must replace the last row of A in order to obtain a singular matrix must be:

$$19.1927 \quad 33.4409 \quad -25.1298 \quad -5.2811$$

CERTIFICATION OF ALGORITHM 43

CROUT II [Henry Thacher, Jr., *Comm. ACM* (1960), 176]

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CROUT II was coded in PUC-R2 and tested in the IBM-1620. Two types of INNERPRODUCT subroutines were used. The first one finds the scalar product in fixed-point arithmetic to increase accuracy, using an accumulator of 32 digits. The second one uses ordinary floating-point with eight significative figures.

Using a unit matrix as right-hand side, a 6×6 segment of Hilbert matrix was inverted. The inverse was inverted again.

The maximum difference between this result and the original segment of Hilbert matrix was:

$$\begin{array}{ll} \text{Using fixed-point INNERPRODUC.} & 8.2426 \times 10^{-4} \\ \text{(Value of determinant)} & 4.7737088 \times 10^{-18} \\ \text{Using floating-point INNERPRODUC.} & 3.014016 \times 10^{-2} \\ \text{(Value of determinant)} & 4.4950721 \times 10^{-18} \end{array}$$

Two typographical errors were observed in the algorithm: