The Crout reduction for sparse matrices

By R. P. Tewarson*

An algorithm is given for minimising the number of non-zero elements created during the forward course of the Crout reduction (no new elements are created in the back substitution). Practical computational techniques for the efficient utilisation of the algorithm are also discussed.

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1. Introduction

Let us consider the solution of the system of equations

$$Ax = b \tag{1.1}$$

where A is a non-singular matrix of order n and x and b are n element column vectors. Let $A^{(k)}$ be the matrix obtained from A after $k-1$ rows and columns of A have been modified by the Crout reduction (Hildebrand, 1956). Let $a_{ij}^{(k)}$ denote the ith row jth column element of $A^{(k)}$. Evidently

$$a_{ij}^{(k)} = a_{ij},\ i, j \geqslant k. \tag{1.2}$$

At the kth stage of the Crout reduction, we can choose any one of the non-zero elements a_{ij}, $i, j \geqslant k$ and move it to the position (k, k)—the north-west corner—by permuting the rows and columns. The row permutations are also applied to the updated right-hand side $b^{(k)}$ at this stage. The column permutations change only the order of the elements of x which should be noted. In any case, the Crout reduction with $a_{kk}^{(k)}$ as the pivot for the kth stage is given by

$$a_{ik}^{(k+1)} = a_{ik}^{(k)} - \sum_{h=1}^{k-1} a_{ih}^{(k)} a_{hk}^{(k)},\ i \geqslant k, \tag{1.3}$$

$$a_{kj}^{(k+1)} = \left(a_{kj}^{(k)} - \sum_{h=1}^{k-1} a_{kh}^{(k)} a_{hj}^{(k)}\right) \Big/ a_{kk}^{(k+1)},\ j > k, \tag{1.4}$$

$$b_k^{(k+1)} = \left(b_k^{(k)} - \sum_{h=1}^{k-1} a_{kh}^{(k)} b_h^{(k)}\right) \Big/ a_{kk}^{(k+1)}. \tag{1.5}$$

If A is sparse then we would like to choose the pivot at the kth stage in such a manner that as few of the elements in (1.3) and (1.4) would change from zero to non-zero. This will minimise not only the storage requirements but also the round-off errors. Computer programs for the Crout reduction, where the sparsity of A is not taken into consideration, are given by Forsythe (1960) and McKeeman (1962).

2. Main result

We will state and prove a theorem which one can use in minimising the local growth of non-zero elements at the kth stage of the Crout reduction (CR). We will need the following definitions. Let S, V and G denote the matrices obtained from the submatrices $a_{ij}^{(k)}$, $i \geqslant k$, $j < k$; $a_{ij}^{(k)}$, $i < k$, $j \geqslant k$ and $a_{ij}^{(k)}$, $i, j \geqslant k$ respectively, by replacing each non-zero element by unity. We define a Boolean matrix D as follows,

$$D = S * V, \tag{2.1}$$

where $*$ denotes Boolean matrix multiplication, viz., the usual matrix multiplication with $1 + 1 = 1$. Let us denote by $\bar{D}$, the matrix obtained from D by changing each zero element to unity and vice-versa, and let

$$W = \bar{D} \oplus G, \tag{2.2}$$

where $\oplus$ denotes Boolean matrix addition, viz., $1+1=1$. If $U = (1, 1, \ldots, 1)$ is an m element vector, where $m = n - k + 1$, then we can define the vectors

$$c = UW \tag{2.3}$$

and

$$r = WU^T, \tag{2.4}$$

where U^T denotes the transpose of U. If r_i and c_j denote the ith and jth elements of r and c respectively then we have the following:

Theorem 2.1

If $r_p + c_q = \max_{i,j} (r_i + c_j)$, and complete cancellation in computing the inner products in (1.3) and (1.4) is neglected, then the choice of $a_{pq}^{(k)}$ as the pivot at the kth stage of CR leads to the creation of minimum number of new non-zero elements.

Proof: Let the ith row and the jth column elements of G, D, $\bar{D}$ and W be denoted by g_{ij}, d_{ij}, $\bar{d}_{ij}$ and w_{ij} respectively. In view of (1.3), (1.4), (2.1), the definitions of S and V: if $d_{ik} = 1$ and $a_{ik}^{(k)} = 0$ then $a_{ik}^{(k+1)} \neq 0$; also if $d_{kj} = 1$ and $a_{kj}^{(k)} = 0$ then $a_{kj}^{(k+1)} \neq 0$. In nearly all the cases this is the only situation when a non-zero element will replace a zero element in CR. It is possible that $d_{ik} = 1$ but $\sum_{h=1}^{k-1} a_{ih}^{(k)} a_{hk}^{(k)} = 0$ or $d_{kj} = 1$ but $\sum_{h=1}^{k-1} a_{kh}^{(k)} a_{hj}^{(k)} = 0$. (Our experience is that such cases are rare for sparse matrices and therefore not included in the analysis given in this note, as it would unnecessarily complicate the analysis without significant advantage.) Thus, neglecting the rare cases when the cancellation of inner product takes place we have $w_{ij} = 0 \Rightarrow \bar{d}_{ij} = 0$ and $g_{ij} = 0 \Rightarrow d_{ij} = 1$ and $g_{ij} = 0 \Rightarrow$ a non-zero element replaces the zero element $a_{ij}^{(k)}$. On the other hand,

$$w_{ij} = 1 \Rightarrow \begin{cases} \bar{d}_{ij} = 0 \text{ and } g_{ij} = 1 \Rightarrow d_{ij} = 1 \text{ and } g_{ij} = 1, \text{ or} \\ \bar{d}_{ij} = 1 \text{ and } g_{ij} = 1 \Rightarrow d_{ij} = 0 \text{ and } g_{ij} = 1, \text{ or} \\ \bar{d}_{ij} = 1 \text{ and } g_{ij} = 0 \Rightarrow d_{ij} = 0 \text{ and } g_{ij} = 0. \end{cases}$$

In all of the three cases given above no new non-zero elements are created. Therefore, in order to minimise

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the number of new non-zero elements created at the kth stage of the CR we choose the pivot $a_{pq}^{(k)}$ such that the row-column pair (p, q) contains the maximum number of the unit elements of W. In other words, $r_p + c_q = \max_{i,j} (r_i + c_j)$, since r_i and c_j denote respectively the total number of ones in the ith row and the jth column of W. This completes the proof of the theorem.

3. Computational considerations

Having chosen $a_{pq}^{(k)}$ as the pivot according to Theorem 2.1, where $r_p + c_q = \max_{i,j} (r_i + c_j)$, the CR is performed using (1.3), (1.4) and (1.5). The pivot is not moved to the position (k, k) but a record of this fact is kept in the computer. To get the W matrix for the $(k + 1)$th stage of the CR we proceed as follows. Let α and β denote respectively, the vectors obtained from the qth column and the pth row of $A^{(k+1)}$ by first deleting the element $a_{pq}^{(k+1)}$ and then replacing the zero elements by unity and the non-zeros by zeros. If $\hat{W}$ is the matrix obtained from W by deleting the pth row and the qth column, then the W matrix associated with the $(k + 1)$th stage of the CR is $\hat{W} \oplus \alpha^* \beta$, the computation of which is fairly easy.

The pivot chosen according to Theorem 3.1 cannot be used due to round-off and stability considerations, in the case that its absolute value is less than a certain chosen number called the *pivot tolerance*. We have found that a pivot tolerance of 10^{-3} worked well in IBM 7040/1401 System (8–9 decimal digits). Thus among all the non-zero elements of $A^{(k)}$, which are not less than the pivot tolerance, we choose as pivot the element with $\max_{i,j} (r_i + c_j)$. If no such element is available, then the element with the maximum absolute value (provided it is greater than 10^{-5}) is chosen as the pivot and Theorem 3.1 is not used at this stage. If even this is not possible then the matrix A is declared singular. For a discussion of pivot and other tolerances in a closely related problem see Clasen (1966). In practice, it is useful to set the numbers that are very small to zero as the computation proceeds e.g., those less than 10^{-7} in absolute value (this is called the *drop tolerance*). Before starting the CR it is recommended that some sort of row-column scaling should be done. A simple method for scaling is given by Forsythe and Moler (1967). More efficient, but complicated, methods are given by Fulkerson and Wolfe (1962), Bauer (1963) and Osborne (1960).

We conclude this note by stating a Theorem (Tewarson 1967, 1968) for the Gaussian Elimination (GE) which corresponds to Theorem 2.1. Let $A^{(k)}$ also denote the square submatrix after $k - 1$ pivot steps have been taken in the GE.

Theorem 3.1

The total number of new non-zero elements that are created in the kth step of the GE if $a_{pq}^{(k)}$ is chosen as a pivot is equal to the corresponding element $\hat{g}_{pq}$ of the matrix $\hat{G}$, where $\hat{G} = G(U^T U - G)G$.

References

Bauer, F. L. (1963). Optimally Scaled Matrices, *Numer. Math.*, Vol. 5, p. 73.

Clasen, R. J. (1966). Techniques for Automatic Tolerance Control in Linear Programming, *Comm. ACM*, Vol. 9, p. 802.

Forsythe, G. E. (1960). Algorithm 16; Crout with Pivoting in ALGOL 60, *Comm. ACM*, Vol. 3, p. 507.

Forsythe, G. E., and Moler, C. B. (1967). *Computer Solution of Linear Algebraic Systems*, Englewood Cliffs, N.J., Prentice Hall, p. 37.

Fulkerson, D. R., and Wolfe, P. (1962). An Algorithm for Scaling Matrices, *SIAM Rev.*, Vol. 4, p. 142.

Hildebrand, F. B. (1956). *Introduction to Numerical Analysis*, New York: McGraw-Hill Inc., p. 429.

McKeeman, W. M. (1962). Algorithm 135; Crout with Equilibration and Iteration, *Comm. ACM*, Vol. 5, p. 553.

Osborne, E. E. (1960). On Pre-Conditioning of Matrices, *J. ACM*, Vol. 7, p. 338.

Tewarson, R. P. (1967). Solution of a System of Simultaneous Linear Equations with Sparse Coefficient Matrix by Elimination Methods, BIT, Vol. 7, p. 226.

Tewarson, R. P. (1968). *The Gaussian Elimination and Sparse Systems*, Stony Brook, N.Y., The College of Engineering Report No. 118. (Presented at the Sparse Matrix Symposium, Sept. 9–10, 1968, Yorktown Heights, N.Y.).

Book Review

Numbers Without End, by C. Lanczos, 1968; 164 pages. (London: *Oliver and Boyd*, 7s. 6d.)

This book has its origin in a series of lectures which the author gave in Indiana about 25 years ago. The audience then were freshmen who were interested in mathematics primarily as a cultural subject, which has played a vital role in the evolution of the human intellect. The author has avoided 'formal algebra' as much as possible in order to bring out the 'real beauty and imaginative features' of the world of numbers. The result is a book on what might reasonably be called 'higher arithmetic', which is the old name for the Theory of Numbers.

The reader is given, in the first half of the book, a very pleasant, gentle introduction to the theory of numbers. including Fermat's theorem, continued fractions and the problem of the period of repeating decimals. In the second half of the book the extension of the rational field to include algebraic numbers and transcendental numbers is discussed and this leads into the question of enumerability of sets. In the last chapter it is proved that the rationals are denumerable and that the reals are not, and various related topics are discussed.

For anyone wishing to have an enjoyable introduction to some beautiful mathematical topics this is a book well worth having.

R. F. Churchhouse (Chilton)