Lecture 11. Math 609 600

The Doolittle factorization.

We want to write

$$A = LU \tag{0.1}$$

where A is an $n \times n$ matrix, L is lower triangular (has zeros above the diagonal), U is upper triangular (has zeros below the diagonal) and $L_{ii} = 1$, for $i = 1, 2, \ldots n$. This is not always possible and we shall provide hypothesis which guarantee a unique factorization of this form below (see Theorem 11.1 below). Such a factorization is called the Doolittle factorization of A.

The point of factorizing a nonsingular matrix $n \times n$ matrix A is that it makes solving the system

$$Ax = b$$

somewhat simpler. Note that if A is nonsingular then so are L and U. Thus, we solve

$$Ax = LUx = b$$

by first solving

$$Ly = b \;\text{ followed by }\; Ux = y$$

by "forward solving" the first and "back solving" the second. Forward solving involves computing $y_1, y_2, \ldots, y_n$ in order while back solving involves computing $x_n, x_{n-1}, \ldots, x_1$ (in the reverse order).

The algorithm for back solving for x above is given by:

Set $x_n = y_n/u_{n,n}$;

For $j = n-1, n-2, \ldots, 1$ do

$$x_j = \left(y_j - \sum_{m=j+1}^{n} u_{j,m} x_m\right) / u_{j,j};$$

enddo

recall $l_{ii}=1$

The matlab code is almost the same but expands the sum using an inner loop:

```
function x=backsolve(U,y,n)

x(n)=y(n)/U(n,n);
```

$l_{11} \cdot y_1 = b_1 \qquad y_1 = \dfrac{b_1}{l_{11}} = b_1$

for $j = 2, \ldots, n$.

$$y_j = \frac{b_j - \sum_{i=1}^{j-1} l_{ji} y_i}{l_{jj}}$$

$$y_j = b_j - \sum_{i=1}^{j-1} l_{ji} y_i$$

end.

$$L = \begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ l_{n1} & \cdots & l_{n,n-1} & l_{nn} \end{bmatrix} \qquad y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad b = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

$$\sum_{i=1}^{j-1} l_{ji} \cdot y_i + l_{jj} \cdot y_j = b_j$$

```
for j=n-1:1:-1
   sum=0;
   for m=j+1:n
      sum=sum+U(j,m)*x(m);
   end
   x(j)=(y(j)-sum)/U(j,j);
end

end
```

The algorithm for forward solving an $n \times n$ lower triangular matrix is left as an exercise. The worst case work estimate for back solving (or forward solving) is roughly the number of non-zeros and is bounded by $O(n^2)$.

This also holds for banded matrices. A banded matrix of bandwidth k has zeros in the i, j entry when $|i - j| > k - 1$ so that $k = 1$ corresponds to a diagonal matrix, $k = 2$ corresponds to a tridiagonal matrix, etc. The work estimate for back solving or forward solving triangular matrices of bandwidth k is $O(nk)$.

For $k = 1, \dots, n$, let A^k denote the principle minor of A, i.e., A^k is the $k \times k$ matrix with entries $A^k_{ij} = A_{ij}$, for $i, j = 1, \dots, k$.

Theorem 11.1. *Suppose that A^k, for $k = 1, 2, \dots n$, is nonsingular, then the Doolittle factorization* (0.1) *of A exists and is unique.*

Proof. Let A be an $n \times n$ matrix whose principle minors, A^k. for $k = 1, 2, \dots, n$ are all nonsingular. The idea is show that there is a unique Doolittle factorization,

$$A^k = L^k U^k \tag{0.2}$$

by mathematical induction. Here L^k and U^k are $k \times k$ with L^k lower triangular, U^k upper triangular and $L^k_{i,i} = 1$, for $i = 1, 2, \dots k$. Of course, if we succeed is developing the sequence of factorizations, then $A = L^n U^n$ is the unique Doolittle factorization of A.

Suppose that $A^1 = (a_{1,1})$ is the 1×1 principle minor of A. Then

$$A^1 = (1)(A_{1,1})$$

is the unique Doolittle factorization of A^1.

Now we assume that for some j with $2 < j \le n$, there is a unique the Doolittle factorization (0.2) for $k = j-1$. We consider the block partitionining of A^j given by

$$A^j = \left(\begin{array}{c|c} A^{j-1} & \alpha^j \\ \hline \beta^j & a_{j,j} \end{array}\right)$$

where $\beta^j = (a_{j,1}, a_{j,2}, \ldots, a_{j,j-1})$ and $\alpha^j = (a_{1,j}, a_{2,j}, \ldots, a_{j-1,j})^t$.

Let $\mathbf{0}$ denote the column vector of length $j-1$. Any Doolittle factorization of A^j must be of the form

$$A^j = L^j U^j = \left(\begin{array}{c|c} L^{j-1} & \mathbf{0} \\ \hline \ell^j & 1 \end{array}\right) \left(\begin{array}{c|c} U^{j-1} & u^j \\ \hline \mathbf{0}^t & u_{j,j} \end{array}\right) \tag{0.3}$$

where

(1) L^{j-1} is lower triangular with 1's on the diagonal,
(2) U^{j-1} is upper triangular,
(3) $\ell^j = (\ell_{j,1}, \ell_{j,2}, \ldots, \ell_{j,j-1})$ is a row vector,
(4) $u^j = (u_{1,j}, u_{2,j}, \ldots, u_{j-1,j})^t$ is a column vector and
(5) $u_{j,j}$ is a number.

Because of the way that block multiplication works, for (0.3) to hold, we must have

$$\begin{aligned} A^j &= \left(\begin{array}{c|c} L^{j-1} & \mathbf{0} \\ \hline \ell^j & 1 \end{array}\right) \left(\begin{array}{c|c} U^{j-1} & u^j \\ \hline \mathbf{0}^t & u_{j,j} \end{array}\right) \\ &= \left(\begin{array}{c|c} L^{j-1}U^{j-1} & L^{j-1}u^j \\ \hline \ell^j U^{j-1} & \ell^j u^j + u_{j,j} \end{array}\right), \end{aligned} \tag{0.4}$$

that is

$$L^{j-1}U^{j-1} = A^{j-1}, \tag{0.5}$$

$$L^{j-1}u^j = \alpha^j, \tag{0.6}$$

$$\ell^j U^{j-1} = \beta^j, \quad \text{and} \tag{0.7}$$

$$\ell^j u^j + u_{j,j} = a_{j,j}. \tag{0.8}$$

It follows from the inductive assumption and (0.5) that $A^{j-1} = L^{j-1}U^{j-1}$ is the unique Doolittle factorization of A^{j-1}. As A^{j-1} is nonsingular, both L^{j-1} and U^{j-1} must also be nonsingular. It then follows from (0.6) that u^j is uniquely determined. Similarly, (0.7) implies that ℓ^j is uniquely determined. Finally, using these results and (0.8) uniquely determines $u_{j,j}$. This completes the proof of the theorem. $\square$

Remark 11.1. *A Crout factorization $A = LU$ is of similar form except that $U_{i,i} = 1$ for $i = 1, 2, \ldots, n$ and no conditions on the diagonal of L are imposed. The Crout factorization exists and is unique under the same conditions as the above therorem.*

Remark 11.2. *Consider the $n \times n$ matrix with entries,*

$$\begin{aligned} A_{1,1} &= 1 \quad \textit{and} \quad A_{n,n} = 1, \\ A_{i,i} &= 2 \quad \textit{for} \quad i = 2, \ldots, n-1, \\ A_{i,i+1} &= A_{i+1,i} = -1, \quad \textit{for} \quad i = 1, 2, \ldots, n-1, \ \textit{and} \\ A_{i,j} &= 0, \quad \textit{when } |i - j| > 1. \end{aligned}$$

We note that A is singular as $A\mathbf{1} = \mathbf{0}$ where $\mathbf{1}$ denotes the n dimensional vector of all 1's. However, for $k < n$, A^k is nonsingular, in fact, A^k is symmetric and positive definite. The proof of the above theorem works for A and yields a unique Doolittle factorization $A = LU$. However, as A is singular U must also be singular, i.e., $u_{n,n} = 0$.

Exercise: Show that LU factorization preserves bandwidth, i.e., if A has bandwidth k, so does L and U. suppose not. Non-zero element at 5

The above exercise is important as reordering the unknowns can reduce the bandwidth. The problem of reordering the unknowns when A is a sparse matrix with large initial bandwidth is well studied. Tim Davis (TAMU computer science) has been involved with sparse direct methods. His program UMFPACK for multifrontal LU factorization has been incorporated into both MATLAB and PYTHON.