MA/CS 522 Fall 2003 Lecture Note 8

Gaussian Elimination and LU Factorization

8.1 Permutation matrix

Definition 8.1 *A* permutation matrix *P is an identity matrix with permuted rows.*

Lemma 8.1 *Let P, P_1, P_2 be permutation matrices, and X be an $n \times n$ matrix. Then*

- *$P^T P = I$, i.e., $P^{-1} = P^T$.*
- $\det(P) = \pm 1$.
- *$P_1 P_2$ is also a permutation matrix.*
- *PX is the same as X with its rows permuted.*
- *XP is the same as X with its columns permuted.*
- *$P_1 X P_2$ reorders both rows and columns of X.*

8.2 Gaussian elimination without pivoting

Theorem 8.1 *The following two statements are equivalent:*

1. *There exists a unique unit lower triangular L and nonsingular upper triangular U such that*
$$A = LU.$$
2. *All leading principal submatrices of A are nonsingular.*

Proof: First show "<u>1 implies 2</u>":

[0]This is for both Lecture 8 and Lecture 9.

$A = LU$ may be partitioned as 2 by 2 block matrices

$$\begin{aligned} \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} &= \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix} \\ &= \begin{bmatrix} L_{11}U_{11} & L_{11}U_{12} \\ L_{21}U_{11} & L_{21}U_{12} + L_{22}U_{22} \end{bmatrix} \end{aligned}$$

where A_{11} is the $j \times j$ leading principal submatrix, as are L_{11} and U_{11}. Therefore

$$\det A_{11} = \det(L_{11}U_{11}) = \det L_{11} \cdot \det U_{11} \neq 0$$

since L_{11} is unit lower triangular and U_{11} is nonsingular and upper triangular.

We now prove "2 implies 1": We do induction on n.

- It is easy for 1-by-1 matrices, $a = 1 \cdot a$.
- Assume it is true for $(n-1)$-by-$(n-1)$ matrices.
- For n-by-n matrix $\tilde{A}$, write

$$\tilde{A} = \begin{bmatrix} A & b \\ c^T & \delta \end{bmatrix} = \begin{bmatrix} L & 0 \\ l^T & 1 \end{bmatrix} \begin{bmatrix} U & u \\ 0 & \eta \end{bmatrix} = \begin{bmatrix} LU & Lu \\ l^T U & l^T u + \eta 1 \end{bmatrix}.$$

By the assumption of induction, unique L and U exist such that $A = LU$. We now need to find unique l, u and η. In fact,

$$u = L^{-1}b, \quad l^T = c^T U^{-1}, \quad \eta = \delta - l^T u,$$

all of which are unique. Finally, note that

$$0 \neq \det(\tilde{A}) = \det(U) \cdot \eta \quad \Rightarrow \quad \eta \neq 0.$$

□

8.3 Gaussian elimination with pivoting

The need of pivoting – mathematical consideration:

The LU factorization can fail on nonsingular matrices, e.g.

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 2 & 1 \\ 2 & 3 & 1 \end{bmatrix},$$

exchanging the first and third rows to get

$$A = \begin{bmatrix} 2 & 3 & 1 \\ 0 & 2 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

This avoids the breakdown in the elimination process. This simple observation is the basis for the Gaussian elimination with pivoting.

Theorem 8.2 *If A is nonsingular, then there exist permutations P_1 and P_2, a unit lower triangular matrix L, and a nonsingular upper triangular matrix U such that*

$$P_1 A P_2 = LU.$$

In fact, one of P_1 and P_2 can be the identity matrix.

Proof: Again, we use the induction on the dimension n.

- When $n = 1$, it is obvious.
- Assume it is true for $n - 1$.
- Now, for n. Since A is nonsingular, it has a nonzero entry. Choose P_1' and P_2' so that (1,1) entry a_{11} of $P_1' A P_2'$ is nonzero[1]

  Write

$$\begin{aligned} P_1' A P_2' &= \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ L_{21} & I \end{bmatrix} \begin{bmatrix} u_{11} & U_{12} \\ 0 & \tilde{A}_{22} \end{bmatrix} \\ &= \begin{bmatrix} u_{11} & U_{12} \\ L_{21} u_{11} & L_{21} U_{12} + \tilde{A}_{22} \end{bmatrix}. \end{aligned} \tag{8.1}$$

  Therefore, we have

$$u_{11} = a_{11} \neq 0, \quad U_{12} = A_{12}, \quad L_{21} = A_{21}/u_{11} = A_{21}/a_{11}$$

  and

$$\tilde{A}_{22} = A_{22} - L_{21} U_{12}.$$

  Note that $\tilde{A}_{22}$ is nonsingular, since

$$0 \neq \pm \det A = \det P_1' A P_2' = \det \begin{bmatrix} 1 & 0 \\ L_{21} & I \end{bmatrix} \cdot \det \begin{bmatrix} u_{11} & U_{12} \\ 0 & \tilde{A}_{22} \end{bmatrix} = u_{11} \cdot \det \tilde{A}_{22}.$$

  By the assumption of the induction, there exist permutations $\tilde{P}_1$ and $\tilde{P}_2$ such that

$$\tilde{P}_1 \tilde{A}_{22} \tilde{P}_2 = \tilde{L} \tilde{U}.$$

  Substituting this into the above 2-by-2 block factorization yields

$$\begin{aligned} P_1' A P_2' &= \begin{bmatrix} 1 & 0 \\ L_{21} & I \end{bmatrix} \begin{bmatrix} u_{11} & U_{12} \\ 0 & \tilde{P}_1^T \tilde{L} \tilde{U} \tilde{P}_2^T \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ L_{21} & I \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P}_1^T \tilde{L} \end{bmatrix} \begin{bmatrix} u_{11} & U_{12} \tilde{P}_2 \\ 0 & \tilde{U} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P}_2^T \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ L_{21} & \tilde{P}_1^T \tilde{L} \end{bmatrix} \begin{bmatrix} u_{11} & U_{12} \tilde{P}_2 \\ 0 & \tilde{U} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P}_2^T \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P}_1^T \end{bmatrix} \begin{bmatrix} 1 & 0 \\ \tilde{P}_1 L_{21} & \tilde{L} \end{bmatrix} \begin{bmatrix} u_{11} & U_{12} \tilde{P}_2 \\ 0 & \tilde{U} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P}_2^T \end{bmatrix}. \end{aligned} \tag{8.2}$$

[1] In fact, we only need one of P_1' and P_2' since nonsingularity of A implies no zero rows and no zero columns.

So let

$$P_1 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P}_1 \end{bmatrix} P_1', \qquad P_2 = P_2' \begin{bmatrix} 1 & 0 \\ 0 & \tilde{P}_2 \end{bmatrix},$$

we have the desired factorization for A

$$P_1 A P_2 = \begin{bmatrix} 1 & 0 \\ \tilde{P}_1 L_{21} & \tilde{L} \end{bmatrix} \begin{bmatrix} u_{11} & U_{12}\tilde{P}_2 \\ 0 & \tilde{U} \end{bmatrix} \equiv LU.$$

□

This proof presents a recursive way of doing the decomposition. Different choices account for different decompositions and numerical performances and stability as well. Two particular ones are in the following definitions.

Definition 8.2 *If we choose $P_2' = I$ and P_1' so that a_{11} is the largest entry in absolute value in its column, and do so recursively afterwards (i.e., at step i of Gaussian elimination, we reorder rows i through n so that the largest entry in the column is on the diagonal). This is* Gaussian elimination with partial (column) pivoting.

Definition 8.3 *Pick P_2' and P_1' so that a_{11} is the largest entry in absolute value in the whole matrix, and do so recursively afterwards (i.e., at step i of Gaussian elimination, we reorder rows and columns i through n so that the largest entry in this submatrix is on the diagonal). This is called* Gaussian elimination with complete pivoting.

8.4 Algorithm

The following algorithm embodies Theorem 8.2. We write the algorithm in a pseudo-programming style.

Algorithm 8.1 (LU factorization with pivoting)

```
for   i = 1 to n − 1
      apply permutations so a_ii ≠ 0
          /* for GEPP, sway rows j and i of A and of computed L,
          for GECP, sway rows j and i of A and computed L and columns k
          and i of A and of computed U, note that j, k ≥ i, see (8.2)*/
      /* compute column i of L (L_21 in (8.1)) */
      for j = i + 1 to n
          l_ji = a_ji / a_ii
      end for
      /* compute row i of U (U_12 in (8.1)) */
      for j = i to n
          u_ij = a_ij
      end for
      /* update A_22 (to get Ã_22 = A_22 − L_21 U_12 in (8.1)) */
      for j = i + 1 to n
          for k = i + 1 to n
               a_jk = a_jk − l_ji * u_ik
          end for
      end for
end for
```

Remarks.

- Note that once column i and row i of A is used, they are never used again. Therefore, it can be used for storing the factors L and U.

- It would be very short to write the above program in Matlab notation.

- One can rederive the above algorithm from scratch starting from the familiar description of Gaussian elimination "Take each row and subtract multiples of it from later rows to zero out entries below the diagonal".

8.5 Solving $Ax = b$ using Gaussian Elimination

Algorithm 8.2 (Gaussian elimination with partial pivoting)

Factorize A into $PA = LU$, where
P: permutation
L: unit lower triangular
U: upper triangular
Permute the entries of b:
$b := Pb$.
Solve $L(Ux) = b$ for Ux by forward substitution:
$Ux = L^{-1}b$.
Solve $Ux = L^{-1}b$ for x by back substitution:
$x = U^{-1}(L^{-1}b)$.

8.6 Operation Count

- **LU factorization**: Replacing loops by summations over the same range, and inner loops by their operation counts in Algorithm 8.1:

$$\sum_{i=1}^{n-1}\left(\sum_{j=i+1}^{n} 1 + \sum_{j=i+1}^{n}\sum_{k=i+1}^{n} 2\right) = \sum_{i=1}^{n-1}\Big((n-i) + 2(n-i)^2\Big) = \frac{2}{3}n^3 + \mathcal{O}(n^2).$$

- **Substitutions:** In Algorithm 8.2: the forward and back substitutions to compute the solution vector x cost only $\mathcal{O}(n^2)$.

- The **total cost** for solving $Ax = b$:

$$\frac{2}{3}n^3 + \mathcal{O}(n^2).$$