MA580H Matrix Computations

Lecture 7: System of Linear Equations-II

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Outline

- Gaussian elimination with pivoting
- Permutated LU decomposition

Pivoting

Consider $\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$. Since the pivot element, that is, $(1,1)$ entry of the matrix is 0, the elimination fails to reduce the matrix to upper triangular form.

However, interchanging the rows we obtain an upper triangular matrix

$$\underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{P} \underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}}_{A} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}}_{U}.$$

The matrix P is a permutation matrix. A permutation matrix is obtained by interchanging rows of identity matrix. The process of interchanging rows is called partial pivoting

Theorem (GEPP): Let A be an $n \times n$ matrix. Then there is a permutation matrix P such that

$$PA = LU$$

where L is unit lower triangular and U is upper triangular.

Gaussian elimination with partial pivoting

Let P_1 be a permutation matrix so that $(1,1)$ entry of P_1A is nonzero. Then for $L_1 := I + \ell_1 e_1^\top$, with $\ell_{i1} := a_{i1}/a_{11}$, $i = 2 : n$, we have

$$L_1^{-1}P_1A = \left[\begin{array}{c|ccc} a_{11} & a_{12} & \cdots & a_{1n} \\ \hline 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} \\ \vdots & \vdots & & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nn}^{(1)} \end{array}\right], \text{ where } a_{ij}^{(1)} = a_{ij} - \ell_{i1}a_{1j}.$$ **Cost:** $2(n-1)^2$ flops.

If $a_{22}^{(1)} = 0$ then elimination breaks down.However, if say $a_{n2}^{(1)} \neq 0$ then we can interchange rows and make $a_{n2}^{(1)}$ as the pivot element and continue elimination.

$$P_2L_1^{-1}P_1A = \left[\begin{array}{c|ccc} a_{11} & a_{12} & \cdots & a_{1n} \\ \hline 0 & a_{n2}^{(1)} & \cdots & a_{nn}^{(1)} \\ \vdots & \vdots & & \vdots \\ 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} \end{array}\right].$$

Here P_2 is the permutation matrix that interchanges second row with n-th row of $L_1^{-1}A$.

Gaussian elimination with partial pivoting

For $L_2 := I + \ell_2 e_2^\top$ with $\ell_{i2} := a_{i2}^{(1)}/a_{n2}^{(1)}$, $i = 3:n$, we have

$$L_2^{-1}P_2L_1^{-1}P_1A = \left[\begin{array}{c|c|cccc} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ \hline 0 & a_{n2}^{(1)} & a_{n3}^{(1)} & \cdots & a_{nn}^{(1)} \\ \hline 0 & 0 & a_{33}^{(2)} & \cdots & a_{3n}^{(2)} \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & a_{n3}^{(2)} & \cdots & a_{nn}^{(2)} \end{array}\right], \quad a_{ij}^{(2)} = a_{ij}^{(1)} - \ell_{i2}a_{2j}^{(1)}. \textbf{ Cost: } 2(n-2)^2 \text{ flops.}$$

Repeating the process we have $L_{n-1}^{-1}P_{n-1}L_{n-2}^{-1}\cdots P_2L_1^{-1}P_1A = U$.
Cost: $2(n-1)^2 + 2(n-2)^2\cdots + 2 \simeq 2n^3/3$ flops.

The matrix $L_{n-1}^{-1}P_{n-1}L_{n-2}^{-1}\cdots P_2L_1^{-1}P_1$ may NOT be lower triangular. However, we show that

$$PA = \underbrace{\hat{L}_1\hat{L}_2\cdots\hat{L}_{n-2}L_{n-1}}_{L}U = LU,$$

where L is unit lower triangular, $\hat{L}_j$'s are obtained from L_j's by permutating their multipliers and $P := P_{n-1}P_{n-2}\cdots P_2P_1$.

GEPP (cont.)

```
    if (A(k,k) ~= 0)
        % compute multipliers for k-th step
        A(k+1:n,k) = A(k+1:n,k)/A(k,k);
        % update A(k+1:n,k+1:n)
        j = k+1:n;
        A(j,j) = A(j,j)-A(j,k)*A(k,j);
    end
end
% strict lower triangle of A, plus I
L = eye(n,n)+ tril(A,-1);
U = triu(A); % upper triangle of A
```

The search for the largest entry in each column guarantees that the denominator `A(k,k)` in the entries `L(k+1:n,k) = A(k+1:n,k)/A(k,k)` is at least as large as the numerators.

This ensures that $|L(i,j)| \leq 1$ for all i, j. This is crucial for stability.

Example

Consider

$$\underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{P_1} \underbrace{\begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix}}_{A} = \begin{bmatrix} 4 & 9 & -3 \\ 2 & 4 & -2 \\ -2 & -3 & 7 \end{bmatrix}.$$

Then $L_1 = I + \begin{bmatrix} 0 \\ \frac{1}{2} \\ -\frac{1}{2} \end{bmatrix} e_1^\top, \quad L_1^{-1}A = \begin{bmatrix} 4 & 9 & -3 \\ 0 & -\frac{1}{2} & -\frac{1}{2} \\ 0 & \frac{3}{2} & \frac{11}{2} \end{bmatrix}$. Now

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}}_{P_2} \begin{bmatrix} 4 & 9 & -3 \\ 0 & -\frac{1}{2} & -\frac{1}{2} \\ 0 & \frac{3}{2} & \frac{11}{2} \end{bmatrix} = \begin{bmatrix} 4 & 9 & -3 \\ 0 & \frac{3}{2} & \frac{11}{2} \\ 0 & -\frac{1}{2} & -\frac{1}{2} \end{bmatrix}.$$

Then $L_2 = I + \begin{bmatrix} 0 \\ 0 \\ -\frac{1}{3} \end{bmatrix} e_2^\top, \quad L_2^{-1}P_2L_1^{-1}P_1A = \begin{bmatrix} 4 & 9 & -3 \\ 0 & \frac{3}{2} & \frac{11}{2} \\ 0 & 0 & \frac{4}{3} \end{bmatrix}$

Example (cont.)

Thus we have $L_2^{-1}P_2L_1^{-1}P_1A = U \Longrightarrow A = MU$, where $M := (L_2^{-1}P_2L_1^{-1}P_1)^{-1} = P_1L_1P_2L_2$. Now

$$\begin{aligned} P_1L_1 &= P_1\begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ -\frac{1}{2} & 0 & 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & 1 & 0 \\ 1 & 0 & 0 \\ -\frac{1}{2} & 0 & 1 \end{bmatrix} \\ P_2L_2 &= P_2\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{1}{3} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{3} & 1 \\ 0 & 1 & 0 \end{bmatrix} \end{aligned}$$

shows that M is not lower triangular. Next, observe that

$$U = L_2^{-1}P_2L_1^{-1}P_1A = L_2^{-1}P_2L_1^{-1}P_2P_2P_1A \Longrightarrow P_2P_1A = P_2L_1P_2L_2U = LU$$

where $L := P_2L_1P_2L_2$ is unit lower triangular. Indeed

$$P_2L_1P_2L_2 = \begin{bmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ \frac{1}{2} & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{1}{3} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{3} & 1 \end{bmatrix}.$$

Permuted LU decomposition ($PA = LU$)

By GEPP we have $L_{n-1}^{-1}P_{n-1}\cdots L_2^{-1}P_2L_1^{-1}P_1A = U$, where P_k is the permutation matrix and $L_k := I + \ell_k e_k^\top$ is the elimination matrix at the k-th step.

Theorem: Set $L(\ell_k) := L_k$. Then

$$P_{n-1}\cdots P_{k+1}L(\ell_k) = L(P_{n-1}\cdots P_{k+1}\ell_k)P_{n-1}\cdots P_{k+1}.$$

Set $\widehat{L}_k := L(P_{n-1}\cdots P_{k+1}\ell_k)$. Then $\widehat{L}_k$ is unit lower triangular and

$$L_{n-1}^{-1}P_{n-1}\cdots L_2^{-1}P_2L_1^{-1}P_1A = L_{n-1}^{-1}\widehat{L}_{n-2}^{-1}\cdots\widehat{L}_2^{-1}\widehat{L}_1^{-1}P_{n-1}\cdots P_1A.$$

Thus, setting $P := P_{n-1}P_{n-2}\cdots P_1$ and $L := \widehat{L}_1\cdots\widehat{L}_{n-2}L_{n-1}$, we have $PA = LU$.

Proof: The first $m-1$ rows of P_m (P_m is used at the m-th step of elimination) are the same as the first $m-1$ rows of I_n. Hence $e_k^\top P_m = e_k^\top$ for $k = 1 : m-1$.

Permuted LU decomposition ($PA = LU$)

Since $e_k^\top P_m = e_k^\top$ for $k = 1 : m-1$, we have
$P_m L(\ell_k) = P_m(I + \ell_k e_k^\top) = P_m + P_m \ell_k e_k^\top = P_m + P_m \ell_k e_k^\top P_m = L(P_m \ell_k) P_m.$

Consequently, $P_{n-1} \cdots P_{k+1} L(\ell_k) = L(P_{n-1} \cdots P_{k+1} \ell_k) P_{n-1} \cdots P_{k+1}.$
Now

$$\begin{aligned} L_3^{-1} P_3 L_2^{-1} P_2 L_1^{-1} P_1 A &= L(-\ell_3) P_3 L(-\ell_2) P_2 L(-\ell_1) P_1 A \\ &= L(-\ell_3) L(-P_3 \ell_2) P_3 P_2 L(-\ell_1) P_1 A \\ &= L(-\ell_3) L(-P_3 \ell_2) L(-P_3 P_2 \ell_1) P_3 P_2 P_1 A. \end{aligned}$$

Continuing this process, we have

$$L_{n-1}^{-1} P_{n-1} \cdots L_2^{-1} P_2 L_1^{-1} P_1 A = L_{n-1}^{-1} \widehat{L}_{n-2}^{-1} \cdots \widehat{L}_2^{-1} \widehat{L}_1^{-1} P_{n-1} \cdots P_1 A.$$

Hence the results follow. $\blacksquare$

Solution of linear system using GEPP

A linear system $Ax = b$ can be solved using GEPP as follows.

$$Ax = b \Longrightarrow PAx = Pb \Longrightarrow LUx = Pb.$$

1. Compute $PA = LU$ ($2n^3/3$ flops)
2. Compute $y = Pb$ (permute the entries of b, no arithmetic needed)
3. Solve $Lz = y$ by forward substitution (n^2 flops)
4. Solve $Ux = z$ by back substitution (n^2 flops).

Total Cost: $\frac{2n^3}{3}$ flops.

GEPP is the standard method used in practice for solving a linear system. GEPP is a default method in MATLAB for solution of a linear system. The command `x = A\b` solves $Ax = b$ using GEPP. The command `[L, U, P] = lu(A)` computes $PA = LU$.

Gaussian elimination with complete pivoting

Gaussian elimination with complete pivoting (GECP) is a variant of GE. At the k-step, GECP searches not just column `A(k:n,k)` but the entire submatrix `A(k:n,k:n)` for the largest entry and then swaps rows and columns to put that entry into `A(k,k)`. After $(k-1)$ steps

$$L_{k-1}^{-1}P_{k-1}\cdots L_1^{-1}P_1AQ_1\cdots Q_{k-1} = \left[\begin{array}{ccc|ccc} * & \cdots & * & * & \cdots & * \\ & \ddots & \vdots & \vdots & \cdots & \vdots \\ & & * & * & \cdots & * \\ \hline & & & a_{kk} & \cdots & a_{kn} \\ & & & \vdots & \ddots & \vdots \\ & & & a_{nk} & \cdots & a_{nn} \end{array}\right].$$

After $n-1$ steps, we have $PAQ = LU$ where P and Q are permutations matrices. If $\mathrm{rank}(A) = r$ then $U = \begin{bmatrix} U_1 & U_2 \\ 0 & 0 \end{bmatrix}$, where U_1 is an $r \times r$ nonsingular upper triangular matrix.

GECP guarantees $|L(i,j)| <= 1$ and $|U(i,j)| <= |U(i,i)|$.

Cost: $2n^3/3 + n^3/3 = n^3$ flops. Additional $n^3/3$ flops is due to finding maximum element at each step.

GEPP versus GECP

- GECP is more expensive ($\mathcal{O}(n^3)$ more operations) than GEPP.
- GECP is usually no more accurate than GEPP which is why GEPP is a default method.
- Examples exist for which GECP does much better than GEPP.
- GEPP and GECP work extremely well in the presence of roundoff.

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