LU Factorization with Partial Pivoting

Before introducing 0s on the kth column (underneath (k,k) entry) swap row k with a row below so that the multipliers are $\leqslant 1$.

* Find $l \in \{k, k+1, \dots, n\}$ such that

$$|a_{lk}^{(k)}| = \max_{j=k,\dots,n} |a_{jk}^{(k)}|$$

* Swap rows k and l:

$$A^{(k)}(k, k:n) \longleftrightarrow A^{(k)}(l, k:n)$$

* Introduce 0s below the (k,k) entry.

Ex

$$A = \begin{bmatrix} 1 & -2 & 1 \\ -4 & 1 & 2 \\ -1 & 4 & 1 \end{bmatrix} \xrightarrow[r_2 \leftrightarrow r_1]{①} \begin{bmatrix} -4 & 1 & 2 \\ 1 & -2 & 1 \\ -1 & 4 & 1 \end{bmatrix}$$

largest in 1.1 on 1st column

$$\xrightarrow[\substack{r_2 + \frac{1}{4}r_1 \\ r_3 - \frac{1}{4}r_1}]{} \begin{bmatrix} -4 & 1 & 2 \\ \frac{-1}{4}\,\cancel{0} & -7/4 & 3/2 \\ \frac{1}{4}\,\cancel{0} & 15/4 & 1/2 \end{bmatrix} =: A^{(2)}$$

largest in 1.1

$$\xrightarrow[r_2 \leftrightarrow r_3]{②} \begin{bmatrix} -4 & 1 & 2 \\ 1/4 & 15/4 & 1/2 \\ -1/4 & -7/4 & 3/2 \end{bmatrix}$$

$$\xrightarrow[r_3 + \frac{7}{15} r_2]{} \begin{bmatrix} -4 & 1 & 2 \\ 1/4 & 15/4 & 1/2 \\ -1/4 & \frac{7}{15}\cancel{0} & 26/15 \end{bmatrix}$$

$$(+) \quad \underbrace{\begin{bmatrix} -4 & 1 & 2 \\ -1 & 4 & 1 \\ 1 & -2 & 1 \end{bmatrix}}_{\substack{\text{obtained} \\ \text{from } A \text{ by} \\ \text{permuting its} \\ \text{rows according}}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 1/4 & 1 & 0 \\ -1/4 & 7/15 & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} -4 & 1 & 2 \\ 0 & 15/4 & 1/2 \\ 0 & 0 & 26/15 \end{bmatrix}}_{U}$$

to ① & ②

Row Interchange Matrices

Matrices obtained from I by swapping two of its rows.

If $I \xrightarrow[r_j \leftrightarrow r_k]{} P$, row interchange matrix

PA swaps rows j and k of A.

e.g.

$$P_{13} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \quad - \text{ swaps rows 1 and 3}$$

(+) can be written as

$$P_2 P_1 A = LU$$

$$P_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$ – corresponds to row swap in 1

$$P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$ – corresponds to row swap in 2

Permutation Matrices

Matrices obtained from I by permuting its rows.

Remarks

(1) A permutation matrix has exactly one nonzero entry which is equal to 1 along every row and column.

(2) A permutation matrix $P \in \mathbb{R}^{n \times n}$ is orthogonal, i.e., $P^T P = P P^T = I$.

(3) Product of row interchange matrices is a permutation matrix.

e.g. $$P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$ is a permutation matrix.

Specification of the algorithm

$$A \xrightarrow[P_1]{} \tilde{A}^{(1)} \xrightarrow[L_1]{} A^{(2)} \xrightarrow[P_2]{} \tilde{A}^{(2)} \xrightarrow[L_2]{} A^{(3)}$$

- P_1 / swap 1st row and a row underneath
- L_1 / introduce 0s on 1st column below (1,1) entry
- P_2 / swap 2nd row and a row underneath
- L_2 / introduce 0s on 2nd column below (2,2) entry

$$\cdots A^{(n-1)} \xrightarrow[P_{n-1}]{} \tilde{A}^{(n-1)} \xrightarrow[L_{n-1}]{} A^{(n)} = U$$

$$P_{n-1} \cdots P_2 P_1 A = L U$$

L – lower triangular matrix (with 1s on the diagonal) consisting of multipliers,

(when k & jth rows are swapped at the kth step, the corresponding multipliers from previous steps must also be swapped.)

Pseudocode

$L \leftarrow I_n$

for $k = 1, \ldots, n-1$

  Find j s.t. $|a_{jk}| = \max_{\ell = k, \ldots, n} |a_{\ell k}|$

  $p(k) \leftarrow j$

  $L(k, 1:k-1) \leftrightarrow L(j, 1:k-1)$, $A(k, k:n) \leftrightarrow A(j, k:n)$

  for $\ell = k+1, \ldots, n$

    $l_{\ell k} \leftarrow a_{\ell k} / a_{kk}$

    $A(\ell, k:n) \leftarrow A(\ell, k:n) - l_{\ell k} A(k, k:n)$

  end

end

$U \leftarrow A$

return

Remarks

(1) $p(k) = j$ means P_k is the row interchange matrix at step k swapping rows k & j.

(2) # of flops is still $\sim 2n^3/3$.

Why the algorithm works

The procedure can be expressed as

$$(L_{n-1}P_{n-1}) \cdots (L_2P_2)(L_1P_1)A = U$$

$$L_j = \begin{bmatrix} I & & \\ & 1 & \\ & -l_{(j+1)j} & \\ & \vdots & I \\ & -l_{nj} & \end{bmatrix}$$

$\downarrow$ jth column

corresponds to introducing 0s below (j,j) entry at the jth step

THM

$$(L_{n-1}P_{n-1}) \cdots (L_1P_1) = (\hat{L}_{n-1} \cdots \hat{L}_1)(P_{n-1} \cdots P_1)$$

where

$$\hat{L}_j = P_{n-1} \cdots P_{j+1} L_j P_{j+1}^{-1} \cdots P_{n-1}^{-1}, \quad j = 1, \ldots, n-2$$

$$\hat{L}_{n-1} = L_{n-1}.$$

Proof

We show

$$(L_{n-1} P_{n-1}) \cdots (L_k P_k) = (\hat{L}_{n-1} \cdots \hat{L}_k)(P_{n-1} \cdots P_k)$$

for $k = n-1, n-2, \cdots, 1$ by induction.

Base case ($k = n-1$)

$$\hat{L}_{n-1} P_{n-1} = L_{n-1} P_{n-1}$$

since $\hat{L}_{n-1} = L_{n-1}$.

Inductive case

Suppose

$$(*)\ (L_{n-1} P_{n-1}) \cdots (L_{k+1} P_{k+1}) = (\hat{L}_{n-1} \cdots \hat{L}_{k+1})(P_{n-1} \cdots P_{k+1}).$$

Let us consider

$$(\hat{L}_{n-1} \cdots \hat{L}_k)(P_{n-1} \cdots P_k) =$$

$$\{\hat{L}_{n-1} \cdots \hat{L}_{k+1}\}(P_{n-1} \cdots P_{k+1} L_k P_{k+1}^{-1} \cdots P_{n-1}^{-1})\{P_{n-1} \cdots P_k\} =$$

$$(\hat{L}_{n-1} \cdots \hat{L}_{k+1})(P_{n-1} \cdots P_{k+1})(L_k P_k).$$

Now by exploiting $(*)$, we have

$$(\hat{L}_{n-1} \cdots \hat{L}_k)(P_{n-1} \cdots P_k) =$$

$$(L_{n-1} P_{n-1}) \cdots (L_{k+1} P_{k+1})(L_k P_k)$$

as desired.

$\square$

Remark: $P_k^{-1} = P_k$.

Closer look at

$$\hat{L}_j = P_{n-1}\cdots P_{j+2}\,P_{j+1}\,L_j\,P_{j+1}\,P_{j+2}\cdots P_{n-1}.$$

suppose P_{j+1} swaps rows $j+1$ and k ($> j+1$)

$$L_j = \begin{array}{r} \\ \\ (j+1)\text{st row} \\ \\ k\text{th row} \\ \\ \end{array}\begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & -l_{(j+1)j} & 1 & & & \\ & \vdots & & \ddots & & \\ & -l_{kj} & & & 1 & \\ & \vdots & & & & \ddots\; 1 \end{bmatrix} \longmapsto \underbrace{\begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & -l_{kj} & & & 1 \\ & \vdots & & & \\ & -l_{(j+1)j} & 1 & & \end{bmatrix}}_{P_{j+1}L_j}$$

jth column (of L_j); $(j+1)$st column, kth colum (of $P_{j+1}L_j$)

$$\longmapsto \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & -l_{kj} & 1 & & \\ & \vdots & & \ddots & \\ & -l_{(j+1)j} & & 1 & \\ & \vdots & & & \ddots\; 1 \end{bmatrix} = P_{j+1}\,L_j\,P_{j+1}$$

Similarly if P_{j+2} swaps rows $j+2$ and $\hat{k}$ ($> j+2$)

$$P_{j+1}\,L_j\,P_{j+1} \longmapsto P_{j+2}\,P_{j+1}\,L_j\,P_{j+1}\,P_{j+2}$$

swaps the multipliers at positions $(j+2, j)$ & $(\hat{k}, j)$.

Hence,

$\hat{L}_j$ is obtained from L_j by swapping the multipliers at the jth step according to row interchanges at steps $j+1, j+2, \ldots, n-1$.

Conclusion

The procedure produces

$$(\hat{L}_{n-1} \cdots \hat{L}_1)(P_{n-1} \cdots P_1) A = U$$

$$\underbrace{(P_{n-1} \cdots P_1)}_{P} A = \underbrace{(\hat{L}_1^{-1} \cdots \hat{L}_{n-1}^{-1})}_{L} U$$

where

$$\hat{L}_j = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -\tilde{\ell}_{(j+1)j} & \ddots & \\ & & \vdots & & \\ & & -\tilde{\ell}_{nj} & & 1 \end{bmatrix}$$

$$\hat{L}_j^{-1} = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & \tilde{\ell}_{(j+1)j} & \ddots & \\ & & \vdots & & \\ & & \tilde{\ell}_{nj} & & 1 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & & & & 0 \\ \tilde{\ell}_{21} & 1 & & & \\ \tilde{\ell}_{31} & \tilde{\ell}_{32} & \ddots & & \\ \vdots & \vdots & & 1 & \\ \tilde{\ell}_{n1} & \tilde{\ell}_{n2} & & \tilde{\ell}_{n(n-1)} & 1 \end{bmatrix}$$

and

$$\begin{bmatrix} \tilde{\ell}_{(j+1)j} \\ \vdots \\ \tilde{\ell}_{nj} \end{bmatrix} \text{ is a permutation of } \begin{bmatrix} \ell_{(j+1)j} \\ \vdots \\ \ell_{nj} \end{bmatrix}$$

according to $P_{j+1}, \ldots, P_{n-1}$.