Pivoting for LU Factorization

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What is Pivoting for LU?

Pivoting for LU factorization is the process of systematically selecting pivots for Gaussian elimination during the LU factorization of a matrix.

Why do we pivot?

- Gaussian elimination is unstable
- Must guarantee no zero pivots

Backward Stability

Definition

An algorithm is stable for a class of matrices C if for every matrix $A \in C$, the computed solution by the algorithm is the exact solution to a nearby problem. Thus, for a linear system problem

$$A\mathbf{x} = \mathbf{b}$$

an algorithm is stable for a class of matrices C if for every $A \in C$ and for each $\mathbf{b}$, it produces a computed solution $\hat{\mathbf{x}}$ that satisfies

$$(A + E)\hat{\mathbf{x}} = \mathbf{b} + \delta\mathbf{b}$$

for some E and $\delta\mathbf{b}$, where $(A + E)$ is close to A and $\mathbf{b} + \delta\mathbf{b}$ is close to $\mathbf{b}$.

Permutation Matrices

- Left multiplication results in row swapping.

$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} = \begin{bmatrix} 7 & 8 & 9 \\ 4 & 5 & 6 \\ 1 & 2 & 3 \end{bmatrix}$$

- We will denote these permutation matrices as P_k where k is the index of the elimination

Permutation Matrices

- Right multiplication results in column swapping.

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 3 & 2 & 1 \\ 6 & 5 & 4 \\ 9 & 8 & 7 \end{bmatrix}$$

- We will denote these matrices as Q_k.

Permutation Matrices

- When computing $PA = LU$,

$$P = P_k P_{k-1} ... P_2 P_1$$

- When computing $PAQ = LU$,

$$Q = Q_1 Q_2 ... Q_{k-1} Q_k$$

LU Factorization

- *LU* factorization in SCLA

$$\begin{bmatrix} -2 & 6 & -8 & 7 & 1 & 0 & 0 & 0 \\ -4 & 16 & -14 & 15 & 0 & 1 & 0 & 0 \\ -6 & 22 & -23 & 26 & 0 & 0 & 1 & 0 \\ -6 & 26 & -18 & 17 & 0 & 0 & 0 & 1 \end{bmatrix} \rightarrow$$

$$\begin{bmatrix} -2 & 6 & -8 & 7 & 1 & 0 & 0 & 0 \\ 0 & 4 & 2 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & -1 & 4 & -1 & -1 & 1 & 0 \\ 0 & 0 & 0 & 2 & -1 & -4 & 2 & 1 \end{bmatrix}$$

LU Factorization

- We will use lower triangular elementary matrices, denoted as M_k, to eliminate entries of A
- Matrix products of permutation and elementary matrices will produce L and U

$$M_1 A = \begin{bmatrix} 1 & 0 & 0 \\ -2/3 & 1 & 0 \\ -1/3 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & 2 & 4 \\ 2 & 1 & 3 \\ 1 & 2 & 4 \end{bmatrix} = \begin{bmatrix} 3 & 2 & 4 \\ 0 & -1/3 & 1/3 \\ 0 & 4/3 & 8/3 \end{bmatrix}$$

Zero Pivots

- The first cause of instability is the situation in which there is a zero in the pivot position

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

- In this case we fail in the first step

Small Pivots

- Small pivots act simlarly to zero pivots

$$A = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 2 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix}, \ U = \begin{bmatrix} 10^{-20} & 1 \\ 0 & 2 - 10^{20} \end{bmatrix}$$

Small Pivots

- The number $2 - 10^{20}$ is not represented exactly but will be rounded to the nearest floating point number which we will say is -10^{20}

$$L' = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix}, \; U' = \begin{bmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{bmatrix}$$

$$L'U' = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 0 \end{bmatrix} \neq A$$

Small Pivots

$$L'U'\hat{\mathbf{x}} = \mathbf{b}$$

$$\mathbf{b} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}, \; \hat{\mathbf{x}} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$A\mathbf{x} = \mathbf{b}$$

$$\mathbf{x} \approx \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Partial Pivoting

- $n \times n$ matrix
- $n - 1$ permutations
- At step k of the elimination, we choose the largest of $n - (k + 1)$ entries of column k as the pivot
- $O(n^2)$

Partial Pivoting - Equations for L and U

- $M'_k = (P_{n-1} \cdots P_{k+1}) M_k (P_{k+1} \cdots P_{n-1})$
- $(M'_{n-1} M'_{n-2} \cdots M'_2 M'_1)^{-1} = L$
- $M_{n-1} P_{n-1} M_{n-2} P_{n-2} \cdots M_2 P_2 M_1 P_1 A = U$

Partial Pivoting

$$B = \begin{bmatrix} \mathbf{x} & x & x & x \\ \mathbf{x} & x & x & x \\ \boldsymbol{\gamma_1} & x & x & x \\ \mathbf{x} & x & x & x \end{bmatrix} \rightarrow \begin{bmatrix} \gamma_1 & x & x & x \\ 0 & \mathbf{x} & x & x \\ 0 & \mathbf{x} & x & x \\ 0 & \boldsymbol{\gamma_2} & x & x \end{bmatrix} \rightarrow$$

$$\begin{bmatrix} \gamma_1 & x & x & x \\ 0 & \gamma_2 & x & x \\ 0 & 0 & \mathbf{x} & x \\ 0 & 0 & \boldsymbol{\gamma_3} & x \end{bmatrix} \rightarrow \begin{bmatrix} \gamma_1 & x & x & x \\ 0 & \gamma_2 & x & x \\ 0 & 0 & \gamma_3 & x \\ 0 & 0 & 0 & x \end{bmatrix}$$

Partial Pivoting - Example

$$A = \begin{bmatrix} 1 & 2 & 4 \\ 2 & 1 & 3 \\ 3 & 2 & 4 \end{bmatrix}$$

$$P_1 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \; P_1 A = \begin{bmatrix} 3 & 2 & 4 \\ 2 & 1 & 3 \\ 1 & 2 & 4 \end{bmatrix}$$

$$M_1 = \begin{bmatrix} 1 & 0 & 0 \\ -2/3 & 1 & 0 \\ -1/3 & 0 & 1 \end{bmatrix}, \; M_1 P_1 A = \begin{bmatrix} 3 & 2 & 4 \\ 0 & -1/3 & 1/3 \\ 0 & 4/3 & 8/3 \end{bmatrix}$$

$$P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \; P_2 M_1 P_1 A = \begin{bmatrix} 3 & 2 & 4 \\ 0 & 4/3 & 8/3 \\ 0 & -1/3 & 1/3 \end{bmatrix}$$

Partial Pivoting - Example

$$M_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1/4 & 1 \end{bmatrix}, \; M_2 P_2 M_1 P_1 A = U = \begin{bmatrix} 3 & 2 & 4 \\ 0 & 4/3 & 8/3 \\ 0 & 0 & 1 \end{bmatrix}$$

$$L = (M_2 P_2 M_1 P_1)^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 1/3 & 1 & 0 \\ 2/3 & -1/4 & 1 \end{bmatrix}$$

Partial Pivoting - Example

$$
\begin{aligned}
PA &= \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 2 & 1 & 3 \\ 3 & 2 & 4 \end{bmatrix} \\
&= \begin{bmatrix} 1 & 0 & 0 \\ 1/3 & 1 & 0 \\ 2/3 & -1/4 & 1 \end{bmatrix} \begin{bmatrix} 3 & 2 & 4 \\ 0 & 4/3 & 8/3 \\ 0 & 0 & 1 \end{bmatrix} \\
&= LU
\end{aligned}
$$

Complete Pivoting

- $n \times n$ matrix
- At step k of the elimination, we scan for the largest value in the submatrix $A_{k:n,k:n}$ to use as the pivot
- $O(n^3)$

Complete Pivoting - Equations for L and U

- $M'_k = (P_{n-1} \cdots P_{k+1}) M_k (P_{k+1} \cdots P_{n-1})$
- $(M'_{n-1} M'_{n-2} \cdots M'_2 M'_1)^{-1} = L$
- $M_{n-1} P_{n-1} M_{n-2} P_{n-2} \cdots M_2 P_2 M_1 P_1 A Q_1 Q_2 \cdots Q_{n-1} = U$

Complete Pivoting

$$B = \begin{bmatrix} \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \boldsymbol{\gamma_1} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \mathbf{x} & \mathbf{x} \end{bmatrix} \to \begin{bmatrix} \gamma_1 & x & x & x \\ 0 & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ 0 & \mathbf{x} & \mathbf{x} & \boldsymbol{\gamma_2} \\ 0 & \mathbf{x} & \mathbf{x} & \mathbf{x} \end{bmatrix} \to$$

$$\begin{bmatrix} \gamma_1 & x & x & x \\ 0 & \gamma_2 & x & x \\ 0 & 0 & \mathbf{x} & \mathbf{x} \\ 0 & 0 & \mathbf{x} & \boldsymbol{\gamma_3} \end{bmatrix} \to \begin{bmatrix} \gamma_1 & x & x & x \\ 0 & \gamma_2 & x & x \\ 0 & 0 & \gamma_3 & x \\ 0 & 0 & 0 & x \end{bmatrix}$$

Complete Pivoting - A Rank Revealing LU Factorization

- Complete pivoting is a rank revealing LU factorization
- Suppose A is a $n \times n$ matrix such that $r(A) = r < n$. At the start of the $r + 1$ elimination, the submatrix $A_{r+1:n,r+1:n} = 0$
- After step r of the elimination, the algorithm can be terminated with the following factorization:

$$PAQ = LU = \begin{bmatrix} L_{11} & 0 \\ L_{21} & I_{n-r} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & 0 \end{bmatrix}$$

Complete Pivoting - Rank Revealing LU Example

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 4 & 6 & 8 \\ 3 & 6 & 9 & 12 \\ 5 & 1 & 2 & 9 \end{bmatrix}$$

- $r(A) = 2$
- At step 2 of the elimination, we get the following factors:

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 3/4 & 1 & 0 & 0 \\ 1/3 & 0 & 1 & 0 \\ 2/3 & 0 & 0 & 1 \end{bmatrix}, \; U = \begin{bmatrix} 12 & 9 & 6 & 3 \\ 0 & \frac{-19}{4} & \frac{-7}{2} & \frac{11}{4} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Rook Pivoting

- $n \times n$ matrix
- At step k of the elimination, we scan the submarix $A_{k:n,k:n}$ for values that are the largest in their respective row and column to use as pivots
- As fast as partial pivoting and as reliable as complete pivoting

Rook Pivoting

$$B = \begin{bmatrix} \mathbf{x} & \mathbf{x} & \mathbf{x} & \gamma \\ \mathbf{x} & \gamma & \mathbf{x} & \mathbf{x} \\ \gamma & \mathbf{x} & \mathbf{x} & \mathbf{x} \\ \mathbf{x} & \mathbf{x} & \gamma & \mathbf{x} \end{bmatrix} \rightarrow \begin{bmatrix} \gamma_1 & x & x & x \\ 0 & \mathbf{x} & \gamma & \mathbf{x} \\ 0 & \gamma & \mathbf{x} & \mathbf{x} \\ 0 & \mathbf{x} & \mathbf{x} & \gamma \end{bmatrix} \rightarrow$$

$$\begin{bmatrix} \gamma_1 & x & x & x \\ 0 & \gamma_2 & x & x \\ 0 & 0 & \mathbf{x} & \gamma \\ 0 & 0 & \gamma & \mathbf{x} \end{bmatrix} \rightarrow \begin{bmatrix} \gamma_1 & x & x & x \\ 0 & \gamma_2 & x & x \\ 0 & 0 & \gamma_3 & x \\ 0 & 0 & 0 & x \end{bmatrix}$$

Rook Pivoting

$$A = \begin{bmatrix} 2 & 10 & 1 & 2 & 4 & 5 \\ 1 & 5 & 2 & 3 & 5 & 6 \\ 3 & 0 & 3 & 1 & 4 & 1 \\ 2 & 2 & 14 & 2 & 1 & 0 \\ 0 & 9 & 5 & 6 & 3 & 8 \\ 1 & 13 & 3 & 4 & 0 & 1 \end{bmatrix}$$

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