

SI231b: Matrix Computations

Lecture 8: Special LU Factorization and Computational Complexity

Yue Qiu

qiuyue@shanghaitech.edu.cn

School of Information Science and Technology
ShanghaiTech University

Oct. 12, 2021

Recap: LU Factorization with Partial Pivoting Through Recursion

For $A \in \mathbb{R}^{n \times n}$, and a permutation matrix P_1

$$P_1 A = \left[\begin{array}{c|c} a_{11}^{(0)} & v^T \\ \hline u & A'_1 \end{array} \right] = \underbrace{\left[\begin{array}{c|c} 1 & 0 \\ \hline 1/a_{11}^{(0)} u & I_{n-1} \end{array} \right]}_{L_1} \underbrace{\left[\begin{array}{c|c} a_{11}^{(0)} & v^T \\ \hline 0 & A'_1 - 1/a_{11}^{(0)} u v^T \end{array} \right]}_{U_1}$$

Then repeat the above procedure to $A'_1 - 1/a_{11}^{(0)} u v^T$, i.e.,

$$\begin{aligned} P'_2 \left(A'_1 - 1/a_{11}^{(0)} u v^T \right) &= \left[\begin{array}{c|c} a_{22}^{(1)} & w^T \\ \hline s & A'_2 \end{array} \right] \\ &= \left[\begin{array}{c|c} 1 & 0 \\ \hline 1/a_{22}^{(1)} s & I_{n-2} \end{array} \right] \left[\begin{array}{c|c} a_{22}^{(1)} & w^T \\ \hline 0 & A'_2 - 1/a_{22}^{(1)} s w^T \end{array} \right] \end{aligned}$$

Denote $P_2 = \begin{bmatrix} 1 & \\ & P'_2 \end{bmatrix}$, we obtain (next page)

Recap: LU Factorization with Partial Pivoting Through Recursion

$$P_2 P_1 A = \underbrace{\begin{bmatrix} 1 & & \\ \frac{1}{a_{11}^{(0)}} P'_2 u & 1 & \\ \frac{1}{a_{11}^{(0)}} P'_2 u & \frac{1}{a_{22}^{(1)}} s & I_{n-2} \end{bmatrix}}_{L_2} \underbrace{\begin{bmatrix} a_{11}^{(0)} & & v^T \\ & a_{22}^{(1)} & w^T \\ & & A'_2 - \frac{1}{a_{22}^{(1)}} s w^T \end{bmatrix}}_{U_2}$$

- ▶ following the above notations, $L = L_{n-1}$, $U = U_{n-1}$
- ▶ P_k only acts on the first $(k-1)$ columns of L_k
- ▶ algorithm style, suitable for computer implementation

Remark:

- ▶ Gaussian elimination tells **why** you can perform an LU factorization, and when does it exist
- ▶ the recursive approach tells **how** you can compute the LU factorization on a modern computer

Example

Please compute an LU factorization with partial pivoting using the method introduced in the last page for

$$\begin{bmatrix} 2 & 4 & 5 \\ -3 & 1 & 4 \\ 4 & 2 & 3 \end{bmatrix}$$

Answer:

$$\begin{bmatrix} & & 1 \\ 1 & & \\ & 1 & \end{bmatrix} \begin{bmatrix} 2 & 4 & 5 \\ -3 & 1 & 4 \\ 4 & 2 & 3 \end{bmatrix} = \begin{bmatrix} 1 & & \\ \frac{1}{2} & 1 & \\ -\frac{3}{4} & \frac{5}{6} & 1 \end{bmatrix} \begin{bmatrix} 4 & 2 & 3 \\ & 3 & \frac{7}{2} \\ & & \frac{10}{3} \end{bmatrix}$$

LU Factorization without Pivoting:

```
U = A, L = I;  
for k = 1 : n-1  
    for j = k+1 : n  
         $\ell_{jk} = u_{jk} / u_{kk}$   
         $u_{j,k:n} = u_{j,k:n} - \ell_{jk} u_{k,k:n}$   
    end  
end  
U = triu(U)
```

Operations count:

► $\mathcal{O}\left(\frac{2}{3}n^3\right)$ flops

Please give your own explanation

LU Factorization with Partial Pivoting:

```
U = A, L = I, P = I;  
for k = 1 : n-1  
    select  $i \geq k$  to maximize  $|u_{ik}|$   
     $u_{k,k:m} \leftrightarrow u_{i,k:m}$  (exchange of rows)  
     $\ell_{k,1:k-1} \leftrightarrow \ell_{i,1:k-1}$   
     $p_{k,:} \leftrightarrow p_{i,:}$   
    for j = k+1 : n  
         $\ell_{jk} = u_{jk} / u_{kk}$   
         $u_{j,k:n} = u_{j,k:n} - \ell_{jk} u_{k,k:n}$   
    end  
end  
U = triu(U)
```

Operations count:

► $\mathcal{O}\left(\frac{2}{3}n^3\right)$ flops, **flops count of partial pivoting?**

LDL^T Factorization for Symmetric Matrices

Theorem

If $A \in \mathbb{R}^{n \times n}$ is symmetric and nonsingular, and every leading principal sub-matrix $A_{\{1, \dots, k\}}$ satisfies

$$\det(A_{\{1, \dots, k\}}) \neq 0,$$

for $k = 1, 2, \dots, n-1$, then there exists a lower-triangular matrix L with unit entries and a diagonal matrix

$$D = \text{diag}(d_1, d_2, \dots, d_n),$$

where $d_i \neq 0$ for $i = 1, 2, \dots, n$, such that $A = LDL^T$. The factorization is unique.

Proof: making use of the LU factorization

Computational complexity: not surprisingly $\mathcal{O}\left(\frac{n^3}{3}\right)$

LDL^T Factorization with Symmetric Pivoting

Symmetry is preferred

If A is symmetric, and P_1 is a permutation matrix

- ▶ $P_1 A$ is not symmetric
- ▶ $P_1 A P_1^T$ is symmetric

Consider the following

$$\begin{aligned} P_1 A P_1^T &= \begin{bmatrix} \alpha & v^T \\ v & A_1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & \\ 1/\alpha v & I_{n-1} \end{bmatrix} \begin{bmatrix} \alpha & \\ & \tilde{A}_1 \end{bmatrix} \begin{bmatrix} 1 & 1/\alpha v^T \\ & I_{n-1} \end{bmatrix}, \end{aligned}$$

with $\tilde{A}_1 = A_1 - 1/\alpha v v^T$ also symmetric.

Note: with symmetric pivoting, α is some diagonal entry a_{ii} , **why?**

When the procedure terminates, $P A P^T = L D L^T$ where

$$P = P_{n-1} \cdots P_2 P_1$$

Symmetric Positive Definite (SPD)

$M = M^T \in \mathbb{R}^{n \times n}$ is SPD iff (if and only if)

$$x^T M x > 0, \quad \forall x \in \mathbb{R}^n \setminus 0$$

Properties of SPD Matrices:

- ▶ real positive eigenvalues
- ▶ positive diagonal entries
- ▶ all principle sub-matrices are SPD
- ▶ $A \in \mathbb{R}^{n \times n}$ is SPD and $X \in \mathbb{R}^{n \times r}$ has full rank, then $X^T A X$ is also SPD

Recursive Factorization

For an SPD matrix $A \in \mathbb{R}^{n \times n}$,

$$\begin{aligned} A &= \begin{bmatrix} a_{11} & w^T \\ w & A_1 \end{bmatrix} \\ &= \underbrace{\begin{bmatrix} \sqrt{a_{11}} & \\ 1/\sqrt{a_{11}}w & I_{n-1} \end{bmatrix}}_{L_1} \underbrace{\begin{bmatrix} 1 & \\ & A_1 - 1/a_{11}ww^T \end{bmatrix}}_{D_1} \underbrace{\begin{bmatrix} \sqrt{a_{11}} & 1/\sqrt{a_{11}}w^T \\ & I_{n-1} \end{bmatrix}}_{L_1^T} \end{aligned}$$

Require: the $(1, 1)$ entry of $(A_1 - 1/a_{11}ww^T)$ should be positive to continue.

Note: $(A_1 - 1/a_{11}ww^T)$ is a principle sub-matrix of $L_1^{-1}AL_1^{-T}$.

Following the same principle, when the procedure terminates,

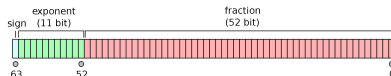
- ▶ $L_n = L$, $D_n = I_n$
- ▶ $A = LL^T$: Cholesky factorization
- ▶ $\mathcal{O}\left(\frac{1}{3}n^3\right)$ flops, half of LU factorization

IEEE Standard for Floating-Point Arithmetic (IEEE 754)

- ▶ single format, 32 bit
- ▶ double format, 64 bit

Take the double format for example,

- ▶ 1 bit for sign;
- ▶ 52 bits for the mantissa;
- ▶ 11 bits for the exponent;



IEEE standard stipulates that each arithmetic operation be correctly rounded, meaning that the computed result is the rounded version of the exact result.

Machine Precision

Resolution is traditionally summarized by a number known as machine epsilon, i.e., ε_m

$$\varepsilon_m = \frac{1}{2} \times (\text{gap between 1 and next largest floating point number})$$

► $\varepsilon_m \approx 5.96 \times 10^{-8}$ for single format

► $\varepsilon_m \approx 1.11 \times 10^{-16}$ for double format

Try the `eps` command in Matlab to get ε_m

Property

$$\forall x \in \mathbb{R}, \text{ there exists } x' \in \mathbb{F}, \text{ such that } |x - x'| < \varepsilon_m |x|$$

where \mathbb{F} represents the set of floating point numbers. Or equivalently,

$$\forall x \in \mathbb{R}, \text{ there exists } \varepsilon \text{ with } |\varepsilon| \leq \varepsilon_m, \text{ such that } fl(x) = x(1 + \varepsilon)$$

Matrix Condition Number

Consider solving the linear equation $Ax = b$ using direct methods, such as LUP/Cholesky factorization, which can be represented by

$$(A + \sigma A)(x + \sigma x) = b.$$

Making use of $Ax = b$ and dropping out the product $\sigma A\sigma x$, we obtain

$$\frac{\|\sigma x\|}{\|x\|} \bigg/ \frac{\|\sigma A\|}{\|A\|} \leq \|A\| \|A^{-1}\|$$

where $\|A\| \|A^{-1}\|$ defines the condition number of the matrix A and is often denoted by $\kappa(A)$.

The linear equation $Ax = b$ is

- ▶ well-conditioned if small σA leads to small σx (small $\kappa(A)$)
- ▶ ill-conditioned if small σA leads to large σx (large $\kappa(A)$)

Note: here the meaning of "small" and "large" depends on the application.

You are supposed to read

- ▶ Gene H. Golub and Charles F. Van Loan. *Matrix Computations*, Johns Hopkins University Press, 2013.

Chapter 2.6 – 2.7, Chapter 4.1 – 4.4

- ▶ Lloyd N. Trefethen and David Bau III. *Numerical Linear Algebra*, SIAM, 1997.

Lecture 12 – 13, 23