4.2 The LU and Cholesky factorizations

Recall : Gaussian elimination for linear system of equations

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ \quad \cdots\cdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n \end{cases}$$

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

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

Issue : One often needs to solve $A\vec{x} = \vec{b}$ w/ one fixed A and many different $\vec{b}$.

Notice: Coeffs in G.e. only depends on A

$\Rightarrow$ do G.e. for A and store info.

$A = A^{(1)}$

$$\left(\begin{array}{cccc:c} \boxed{a_{11}} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array}\right) \begin{array}{c} ① \\ ② \\ \vdots \\ ⓝ \end{array}$$

Suppose $a_{11} \neq 0$. Then, row operations:

$$ⓘ \longrightarrow ⓘ - \frac{a_{i1}}{a_{11}} ① \qquad i = 2, \cdots, n$$

$A^{(2)}$

$$\left(\begin{array}{cccc:c} a_{11}^{(2)} & a_{12}^{(2)} & \cdots & a_{1n}^{(2)} & b_1^{(2)} \\ 0 & \boxed{a_{22}^{(2)}} & \cdots & a_{2n}^{(2)} & b_2^{(2)} \\ \vdots & \vdots & & & \vdots \\ 0 & a_{n2}^{(2)} & \cdots & a_{nn}^{(2)} & b_n^{(2)} \end{array}\right)$$

$$A^{(2)} = M^{(1)} A^{(1)}$$

$$M^{(1)} = \begin{pmatrix} 1 & & & \\ -\frac{a_{21}}{a_{11}} & 1 & & \\ \vdots & & \ddots & \\ -\frac{a_{n1}}{a_{11}} & & & 1 \end{pmatrix}$$

Suppose $a_{22}^{(2)} \neq 0$. Then

$$ⓘ \rightsquigarrow ⓘ - \frac{a_{i2}^{(2)}}{a_{22}^{(2)}} ② \qquad i = 3, \cdots, n$$

$$\vdots$$

(total $n-1$ steps)

$$\left(\begin{array}{cccc|c} a_{11}^{(n)} & a_{12}^{(n)} & \cdots & a_{1n}^{(n)} & b_1^{(n)} \\ & a_{22}^{(n)} & \cdots & a_{2n}^{(n)} & b_2^{(n)} \\ & & \ddots & \vdots & \vdots \\ & & & a_{nn}^{(n)} & b_n^{(n)} \end{array}\right)$$

$A^{(n)}$

(upper-triangular form)

$$A^{(3)} = M^{(2)} A^{(2)}$$

$$M^{(2)} = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & -\frac{a_{32}^{(2)}}{a_{22}^{(2)}} & 1 & & \\ & \vdots & & \ddots & \\ & -\frac{a_{n2}^{(2)}}{a_{22}^{(2)}} & & & 1 \end{pmatrix}$$

$$\vdots$$

$$U := A^{(n)} = M^{(n-1)} A^{(n-1)}$$

Backward substitution:

$$x_n = \frac{b_n^{(n)}}{a_{nn}^{(n)}}$$

$$x_{n-1} = \frac{1}{a_{n-1,n-1}^{(n)}} \left(b_{n-1}^{(n)} - a_{n-1,n}^{(n)} x_n \right)$$

$$\vdots$$

$$x_1 = \frac{1}{a_{11}^{(n)}} \left(b_1^{(n)} - a_{12}^{(n)} x_2 - \cdots - a_{1n}^{(n)} x_n \right)$$

$$U = M^{(n-1)} \cdots M^{(2)} M^{(1)} A$$

$$A = \underbrace{(M^{(1)})^{-1} (M^{(2)})^{-1} \cdots (M^{(n-1)})^{-1}}_{:= L} U$$

$:= L$ (lower-triangular w/ diagonal entries 1)

$$\begin{pmatrix} 1 & & & \\ \wr & 1 & & \\ \wr & & \ddots & \\ \wr & & & 1 \end{pmatrix} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & \wr & \ddots & \\ & \wr & & 1 \end{pmatrix} \cdots$$

$$L = \begin{pmatrix} 1 & & & & \\ \frac{a_{21}}{a_{11}} & 1 & & & \\ \frac{a_{31}}{a_{11}} & \frac{a_{32}^{(2)}}{a_{22}^{(2)}} & 1 & & \\ \vdots & \vdots & & \ddots & \\ & & & & 1 \\ \frac{a_{n1}}{a_{11}} & \frac{a_{n2}^{(2)}}{a_{22}^{(2)}} & \cdots & \frac{a_{n,n-1}^{(n-1)}}{a_{n-1,n-1}^{(n-1)}} & 1 \end{pmatrix}$$

Def For an $n \times n$ matrix A, an LU-decomposition (LU-factorization) is $A = LU$ w/ L lower-triangular and U upper-triangular.

(usually one requires A nonsingular, so L, U nonsingular, i.e. diagonal entries of L, U are nonzero).

Suppose we have an LU-decomposition of A. Then, to solve $A\vec{x} = \vec{b}$,

$$L \underbrace{U \vec{x}}_{\vec{y}} = \vec{b} \qquad \begin{cases} L\vec{y} = \vec{b} \\ U\vec{x} = \vec{y} \end{cases}$$

$$\begin{pmatrix} l_{11} & & & \\ l_{12} & l_{22} & & \\ \vdots & & \ddots & \\ l_{1n} & l_{2n} & \cdots & l_{nn} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

forward substitution

$$y_1 = \frac{b_1}{l_{11}}$$

$$y_2 = \frac{1}{l_{22}}(b_2 - l_{12} y_1)$$

$$\cdots$$

$$y_n = \frac{1}{l_{nn}}(b_n - l_{1n} y_1 - \cdots - l_{n-1,n} y_{n-1})$$

$U\vec{x} = \vec{y}$ can be solved by backward substitution.

- Computational cost of G.e. / LU-decomp.

LU-decomp. :

Step 1 : $(n-1)+(n-1)^2 \simeq n^2$

Step 2 : $(n-1)^2$

$\vdots$

Step $n-1$: 1^2

$$1^2+2^2+\cdots+n^2 \approx \frac{1}{3}n^3$$

backward / forward substitution :

$$1+2+\cdots+n \approx \frac{1}{2}n^2$$

$\Rightarrow$ If we do LU-decomp. for A and solve $A\vec{x}=\vec{b}$ m times, then

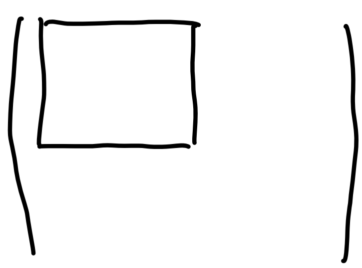
$$\text{total cost} = \frac{1}{3}n^3 + m\cdot n^2$$

Thm If all leading minors of A are nonsingular, then A has an LU-decomposition.

$$\begin{vmatrix} a_{11} & \cdots & a_{1k} \\ \vdots & & \vdots \\ a_{k1} & \cdots & a_{kk} \end{vmatrix} \quad k=1,\cdots,n$$

Proof

The property "all leading minors are nonsingular" is preserved by Gaussian elimination.



$\Rightarrow$ before Step k,

Since the k-th leading minor here is upper-triangular and nonsingular, we have $a_{kk}^{(k)} \neq 0$.

$\Rightarrow$ G.e. can always be done, giving LU-decomp.

Thm LU-decomp. is unique once the diagonal entries of L is given.

$$LU \qquad (LD)(D^{-1}U)$$

Proof Suppose $A = LU = \tilde{L}\tilde{U}$ w/ $L, \tilde{L}$ having the same diagonal.

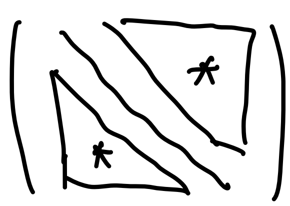
$$\Rightarrow \underbrace{\tilde{L}^{-1}L}_{\text{lower-triangular}} = \underbrace{\tilde{U}U^{-1}}_{\text{upper-triangular}} \qquad \Rightarrow \tilde{L}^{-1}L \text{ is diagonal.}$$

$$L = \begin{pmatrix} l_{11} & & \\ \vdots & \ddots & \\ \cdots & \cdots & l_{nn} \end{pmatrix} \qquad \tilde{L} = \begin{pmatrix} l_{11} & & \\ \vdots & \ddots & \\ \cdots & \cdots & l_{nn} \end{pmatrix} \qquad \tilde{L}^{-1} = \begin{pmatrix} l_{11}^{-1} & & \\ \vdots & \ddots & \\ \cdots & \cdots & l_{nn}^{-1} \end{pmatrix}$$

$$\tilde{L}^{-1}L = \begin{pmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{pmatrix} = I \qquad \Rightarrow \tilde{L} = L, \quad \tilde{U} = U.$$

LU-decomp for symmetric matrices

Assume A is symmetric, and has an LU-decomp. w/ L having diagonal entries 1.

$A =$ 

$$A = \boxed{LU} = LD\tilde{U}$$

where $D = \mathrm{diag}\{u_{11}, \cdots, u_{nn}\}$ and $\tilde{U}$ is upper-triangular w/ diag. entries 1

$$D^{-1}U = \begin{pmatrix} 1 & * \\ & \ddots \\ & & 1 \end{pmatrix} := \tilde{U}$$

$$A^T = A = \boxed{\underbrace{\tilde{U}^T}_{\substack{\text{lower}\\\text{triangular}}} \underbrace{DL^T}_{\substack{\text{upper-}\\\text{triangular.}}}}$$

$\Rightarrow$ by uniqueness of LU-decomp., $\tilde{U}^T = L$

$\Rightarrow A = LDL^T$

Therefore, for sym. matrices, one only needs to store $\underset{\frac{1}{2}n(n-1)}{\underset{\uparrow}{L}}$ and $\underset{n}{\underset{\uparrow}{D}}$ for its LU-decomp.

(about half of the cost for general matrix).

- When doing G.e. for sym. matrix,

$$\begin{pmatrix} \boxed{a_{11}} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \text{Sym}$$

$$a_{32}^{(2)} = a_{32} - \frac{a_{31}}{a_{11}} a_{12}$$

$$a_{23}^{(2)} = a_{23} - \frac{a_{21}}{a_{11}} a_{13}$$

$$ⓘ \rightsquigarrow ⓘ - \frac{a_{i1}}{a_{11}} ① \qquad i = 2, \cdots, n$$

$$\begin{pmatrix} a_{11}^{(2)} & a_{12}^{(2)} & \cdots & a_{1n}^{(2)} \\ 0 & \boxed{a_{22}^{(2)}} & \cdots & a_{2n}^{(2)} \\ \vdots & \vdots & & \\ 0 & a_{n2}^{(2)} & \cdots & a_{nn}^{(2)} \end{pmatrix} \text{Sym}$$

you only need to calculate lower-triangular and diagonal parts for these entries

$\Rightarrow$ Save about half of the computational cost of G.e.