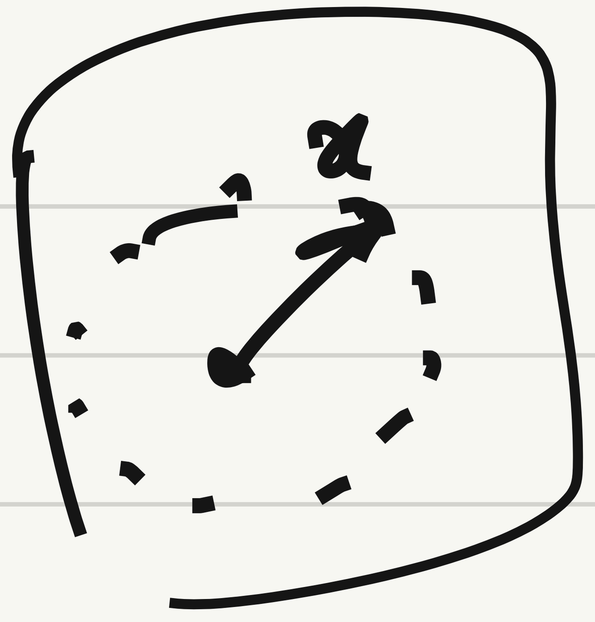
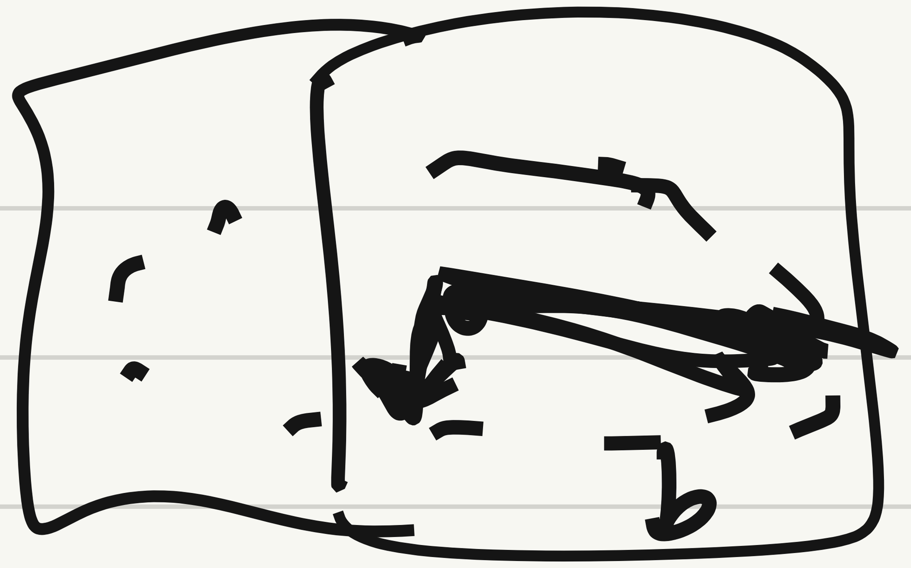
COL726: ~~LU factorization~~





$A \in \mathbb{C}^{m\times n}$, $\vec{b} \in \mathbb{C}^{m}$

solve $\min_{\vec{x}} \|\vec{b} - A\vec{x}\|$ using QR factorization : backward stable

<u>Conditioning of linear systems & least squares problems</u>

$A \in \mathbb{C}^{m\times m}$, $\vec{b} \in \mathbb{C}^{m}$, solve $A\vec{x} = \vec{b}$

equiv. to $\vec{x} = A^{-1}\vec{b}$

$\sup \|A^{-1}\delta b\| / \|\delta b\|$

Cond. num. of $\vec{x}$ w.r.t. $\vec{b}$: $\kappa_{\vec{b}\to\vec{x}} = \sup_{\delta b} \dfrac{\|\delta\vec{x}\| / \|\delta\vec{b}\|}{\|\vec{x}\| / \|\vec{b}\|} = \dfrac{\|A^{-1}\|\,\|\vec{b}\|}{\|\vec{x}\|} \leq \kappa(A)$

$\kappa(A) = \|A\|\,\|A^{-1}\| = \sigma_1/\sigma_n$

Define $\eta = \dfrac{\|A\|\,\|\vec{x}\|}{\|\vec{b}\|} \in [1, \kappa(A)]$

$$\eta = \frac{\|A\|\,\|x\|}{\|b\|} \to \frac{\|b\|}{\|x\|} = \|A\|/\eta \to \kappa_{b\to x} = \frac{\|A^{-1}\|\,\|b\|}{\|x\|} = \frac{\|A\|\,\|A^{-1}\|}{\eta} = \boxed{\frac{\kappa(A)}{\eta}}$$

$$\boxed{\kappa_{A\to \vec{x}} = \kappa(A)}$$

$$\|A\|\,\|A^{-1}\|$$

$$\vec{x} = A^{-1}\vec{b}$$

$$\vec{x} + \delta\vec{x} = (A + \delta A)^{-1}\vec{b}$$

$$(A + \delta A)(\vec{x} + \delta\vec{x}) = \vec{b}$$

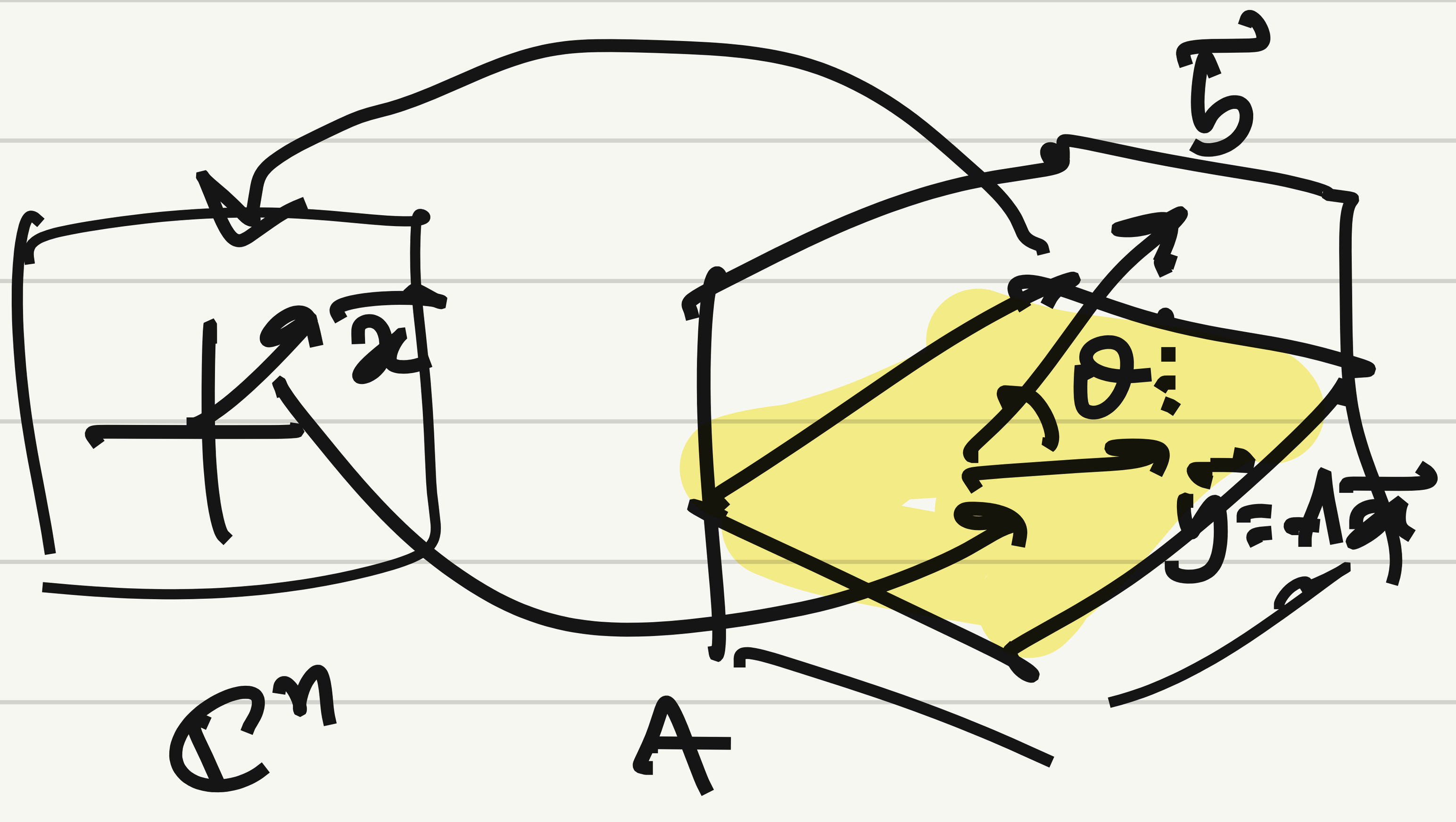
$$\cancel{A\vec{x}} + A\,\delta\vec{x} + \delta A\,\vec{x} + \underbrace{\cancel{\delta A\,\delta\vec{x}}}_{0} = \cancel{\vec{b}}$$

$$A\,\delta\vec{x} + \delta A\,\vec{x} = 0$$

$$\delta\vec{x} = -A^{-1}\,\delta A\,\vec{x} \to \frac{\|\delta\vec{x}\|}{\|\vec{x}\|} \le \|\delta A\|\,\|A^{-1}\| = \overbrace{\|A\|\,\|A^{-1}\|}^{\kappa(A)} \cdot \frac{\|\delta A\|}{\|A\|}$$

Conditioning of least-squares problems

$$\min_{\vec{x}} \|\vec{b} - A\vec{x}\|$$



$$\kappa(A) = \|A\|\,\|A^+\| = \sigma_1/\sigma_n$$

$$\eta = \frac{\|A\|\,\|\vec{x}\|}{\|A\vec{x}\|} \in [1, \kappa(A)]$$

$$\cos\theta = \frac{\|A\vec{x}\|}{\|\vec{b}\|} \in [0, 1]$$

$$\kappa_{\vec{b} \to \vec{x}} = \frac{\kappa(A)}{\eta \cos\theta}$$

$$\kappa_{A \to \vec{x}} \leq \kappa(A) + \underbrace{\frac{\kappa(A)^2 \tan\theta}{\eta}}$$

$$\frac{\|\tilde{x} - x\|}{\|x\|} = O(\kappa_{A\to x}\,\varepsilon_m)$$

Conditioning of lsq. problems is especially bad if:

$b \perp \text{range}(A)$ $\quad (\cos\theta \approx 0)$

or $\|A\vec{x}\| \approx \|A\| \cdot \|x\|$ $\quad (\eta \approx 1)$

LU factorization

$A \in \mathbb{C}^{m\times m}$, $\vec{b} \in \mathbb{C}^m$, solve $A\vec{x} = \vec{b}$

Bad!

~~1.~~ Compute A^{-1}, then $\vec{x} = A^{-1}\vec{b}$ ←

2. $[\,A \mid \vec{b}\,]$

$$A = \begin{bmatrix} 1.00 & 2.01 \\ 1.01 & 2.03 \end{bmatrix}, \quad \vec{b} = \begin{bmatrix} 1.01 \\ 1.02 \end{bmatrix}$$

$$\vec{x} = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

$$A^{-1} = \begin{bmatrix} -2.03\times 10^4 & 2.01\times 10^4 \\ 1.01\times 10^4 & 1.00\times 10^4 \end{bmatrix}$$

$$\tilde{x} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$[A \mid \vec{b}] = \left[\begin{array}{cc|c} 1.00 & 2.01 & 1.01 \\ 1.01 & 2.03 & 1.02 \end{array}\right]$$

$$= \left[\begin{array}{cc|c} 1.00 & 2.01 & 1.01 \\ 0 & * & * \end{array}\right]$$

If we have fixed matrix A but many different $\vec{b}_1, \vec{b}_2, \dots$

$A = QR \leftarrow O(n^3)$

$QR\vec{x} = \vec{b} \leftarrow O(n^2)$

$$\overbrace{L_{m-1}\cdots L_2 L_1 A} = \overbrace{U}$$

$$A = \underbrace{(L_{m-1}\cdots L_2 L_1)^{-1}}_{L}\, U$$

lower triangular

$$A = LU$$

upper triangular

solve $L\underbrace{Ux} = b$

"triangular triangularization"

$$A = \begin{bmatrix} \boxed{a_{11}} & a_{12} & \cdots \\ a_{21} & \cdots & \\ a_{31} & \cdots & \\ \vdots & & \end{bmatrix} = \begin{bmatrix} \vec{a}_1^{\,*} \\ \hline \vec{a}_2^{\,*} \\ \hline \vec{a}_3^{\,*} \\ \hline \vdots \end{bmatrix} \xrightarrow{L_1} \underbrace{\begin{bmatrix} \vec{a}_1^{\,*} \\ \hline \vec{a}_2^{\,*} - \frac{a_{21}}{a_{11}} \vec{a}_1^{\,*} \\ \hline \vec{a}_3^{\,*} - \frac{a_{31}}{a_{11}} \vec{a}_1^{\,*} \\ \hline \vdots \end{bmatrix}}_{L_1 A}$$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ \hline -\frac{a_{21}}{a_{11}} & 1 & 0 & \cdots & 0 \\ \hline -\frac{a_{31}}{a_{11}} & 0 & 1 & \cdots & 0 \\ \hline \vdots & & & \ddots & \\ & & & & 1 \end{bmatrix}}_{L_1}$$

$$A \to L_1 A \to \underbrace{L_2 L_1}_{\text{lower tri}} A \to \cdots \to \underbrace{L_{m-1} \cdots L_2 L_1}_{L^{-1}} A = U$$

$$L = L_1^{-1} L_2^{-1} \cdots L_{m-1}^{-1}$$

What is L_1^{-1}?

$$\underbrace{\begin{bmatrix} 1 & & & & \\ -l_{21} & 1 & & & \\ -l_{31} & & 1 & & \\ \vdots & & & \ddots & \\ -l_{m1} & & & & 1 \end{bmatrix}}_{L_1^{-1}} \underbrace{\begin{bmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ l_{31} & & 1 & & \\ \vdots & & & \ddots & \\ l_{m1} & & & & 1 \end{bmatrix}}_{L_1} = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}$$

$$L_1^{-1} L_2^{-1} = \underbrace{\begin{bmatrix} 1 & & & & \\ -l_{21} & 1 & & & \\ -l_{31} & & 1 & & \\ \vdots & & & \ddots & \\ -l_{m1} & & & & 1 \end{bmatrix}}_{L_1^{-1}} \underbrace{\begin{bmatrix} 1 & & & \\ & 1 & & \\ & -l_{32} & 1 & \\ & \vdots & & \ddots \\ & -l_{m2} & & & 1 \end{bmatrix}}_{L_2^{-1}} = \underbrace{\begin{bmatrix} 1 & & & & \\ -l_{21} & 1 & & & \\ -l_{31} & -l_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ -l_{m1} & -l_{m2} & & & 1 \end{bmatrix}}_{L_1^{-1} L_2^{-1}}$$

$$L = \begin{bmatrix} 1 & & & & \\ \bullet & 1 & & & \\ \bullet & \bullet & 1 & & \\ \vdots & \vdots & \vdots & \ddots & \\ \bullet & \bullet & \cdots & & 1 \end{bmatrix}$$

Algo:

$L = I, \quad U = A$

for each $k = 1 \ldots m-1$

  for each $j = j+1 \ldots m$

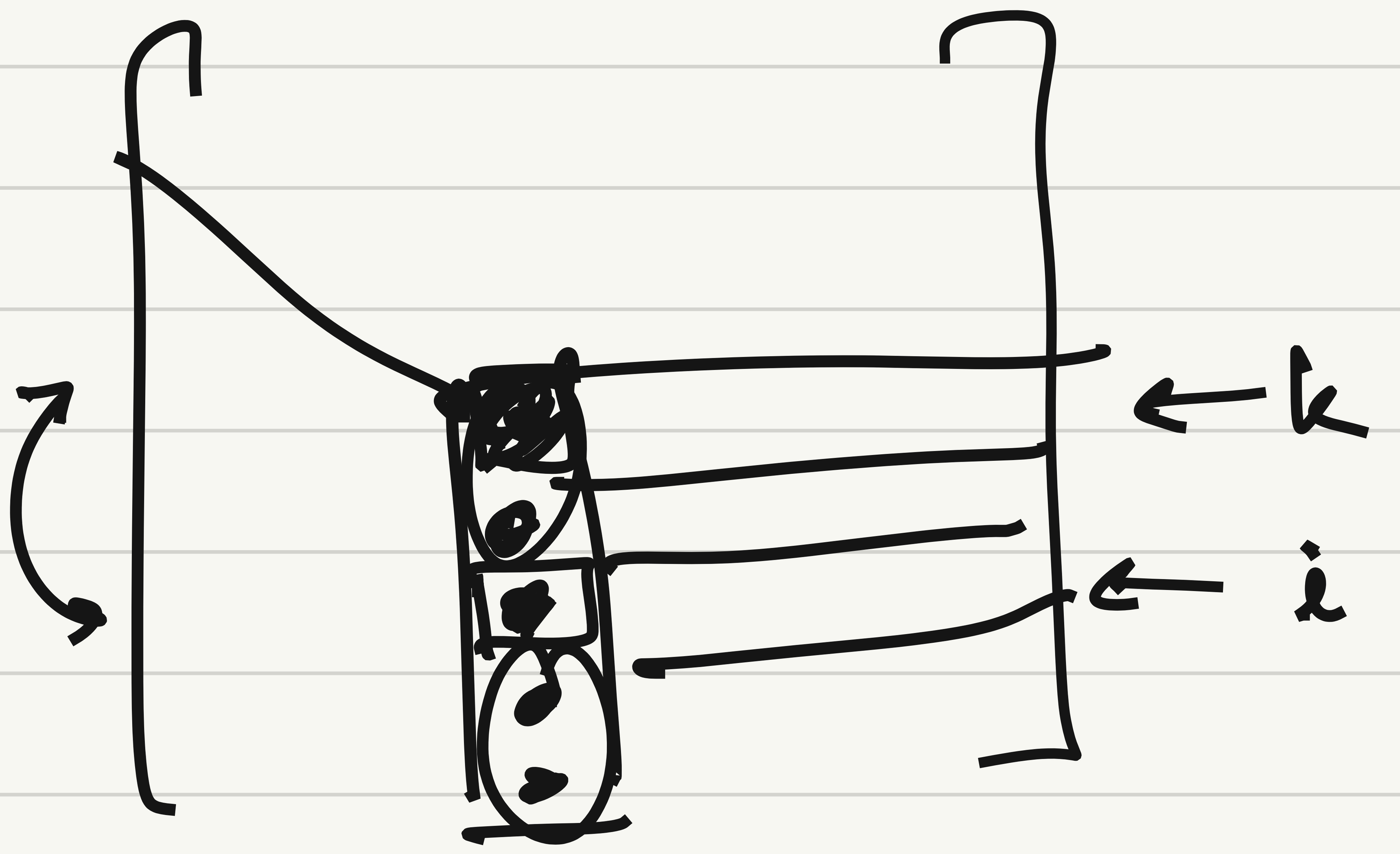
    row $\vec{u}_j \mathrel{-}= u_{jk}/u_{kk} \cdot \vec{u}_k$

    record $l_{jk} = u_{jk}/u_{kk}$

operation count $\sim \frac{2}{3} m^3$ flops

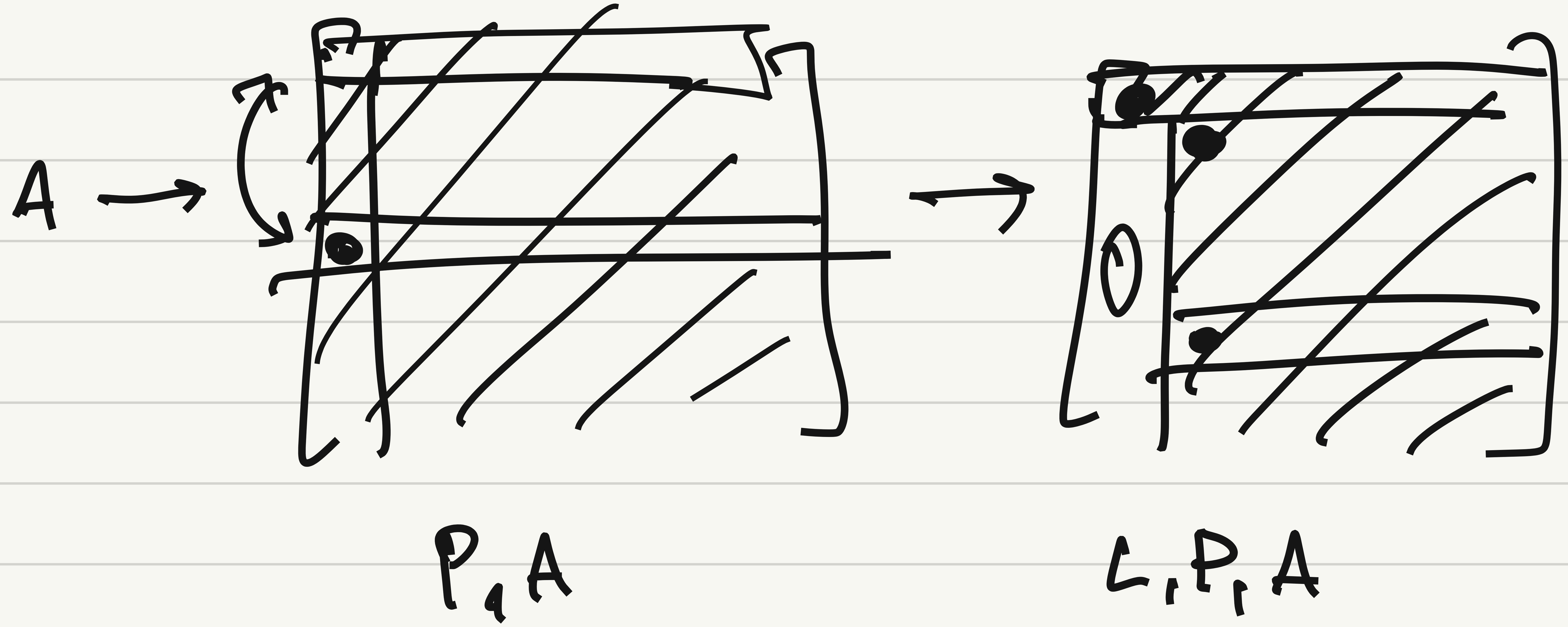
$$A = \begin{bmatrix} 10^{-12} & 1 \\ 1 & 0 \end{bmatrix}$$

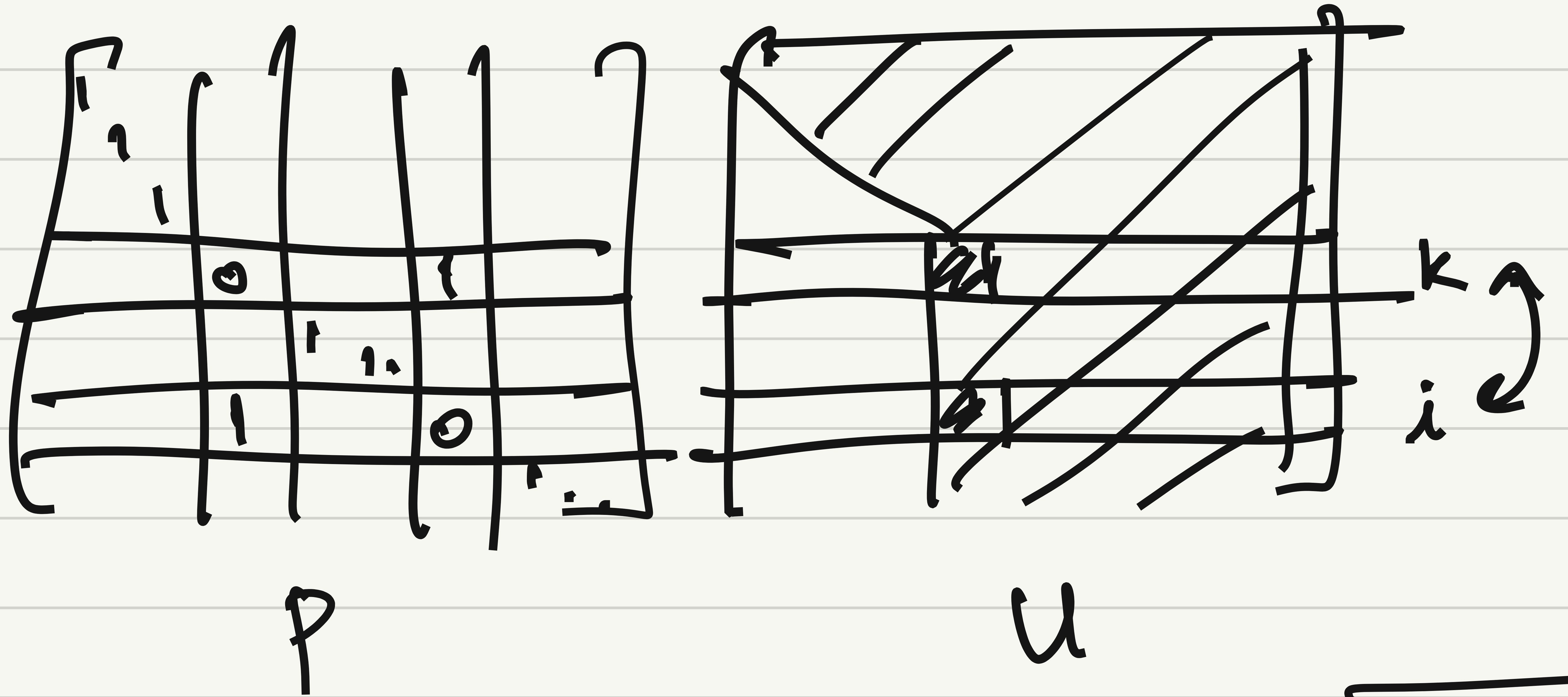
If diag. entry u_{kk} is v. small $\Rightarrow$ instability



Always pick largest entry (in absolute value).

Swap that row into current row : $\boxed{\text{pivoting}}$



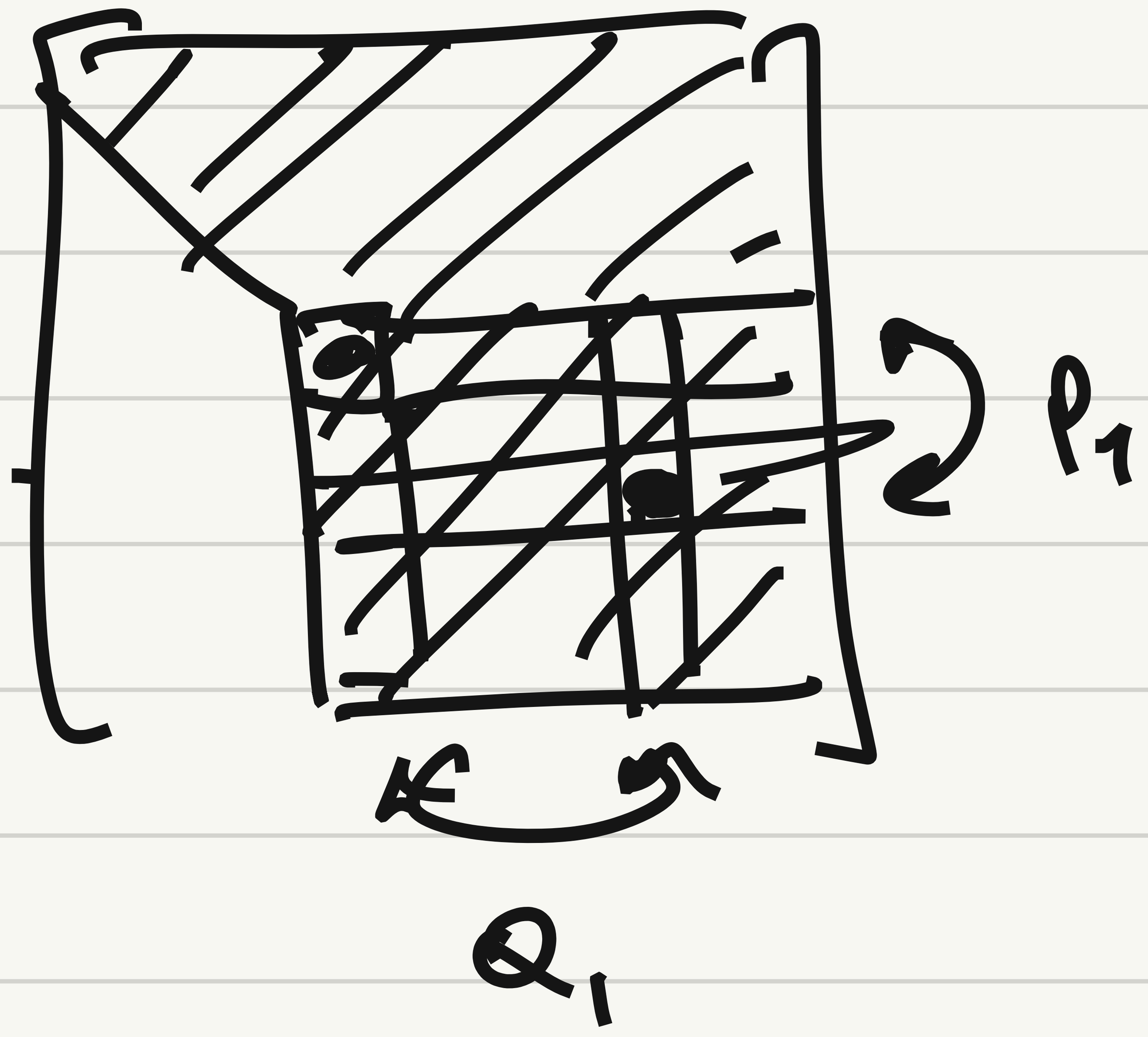


$\rightarrow L_2 P_2 L_1 P_1 A \rightarrow \cdots \rightarrow$

$\rightarrow L_{m-1} P_{m-1} \cdots L_1 P_1 A = U$

$\boxed{\text{partial pivoting}}$

Swap rows $= P_1 A$



swap cols $= A Q_1$

$\cdots L_1 P_1 A Q_1 \cdots$: $\boxed{\text{complete pivoting}}$: rarely worth the effort

Partial pivoting: $\underbrace{L_{m-1} P_{m-1} \cdots L_2 P_2 L_1 P_1}_{\neq L^{-1}} A = U$

$\boxed{\text{LU factorization}}$

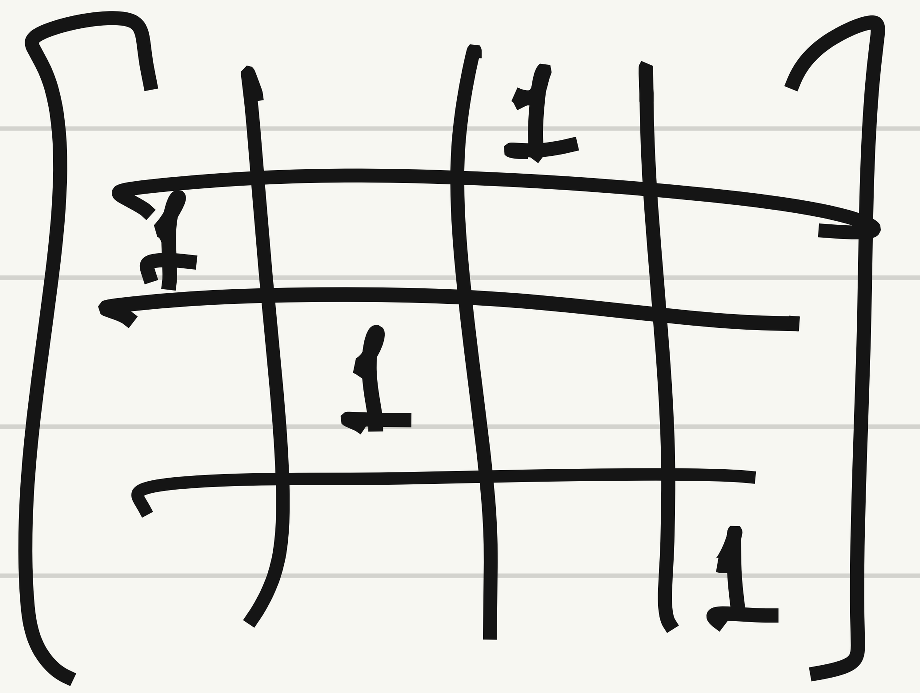
$PA = LU$

$L_2 P_2 L_1 P_1 A = L_2 L_1' P_2 P_1 A \to \cdots \to \underbrace{L'_{m-1} \cdots L'_2 L'_1}_{L^{-1}} \underbrace{P_{m-1} \cdots P_2 P_1}_{P} A = U$

we will find

$P = P_{m-1} \cdots P_2 P_1$: $\boxed{\text{permutation matrix}}$ = any matrix with exactly one 1 in each row & each col., rest 0.

$\Rightarrow$ permutation matrices are unitary / orthogonal



$PA = \underbrace{L}U$

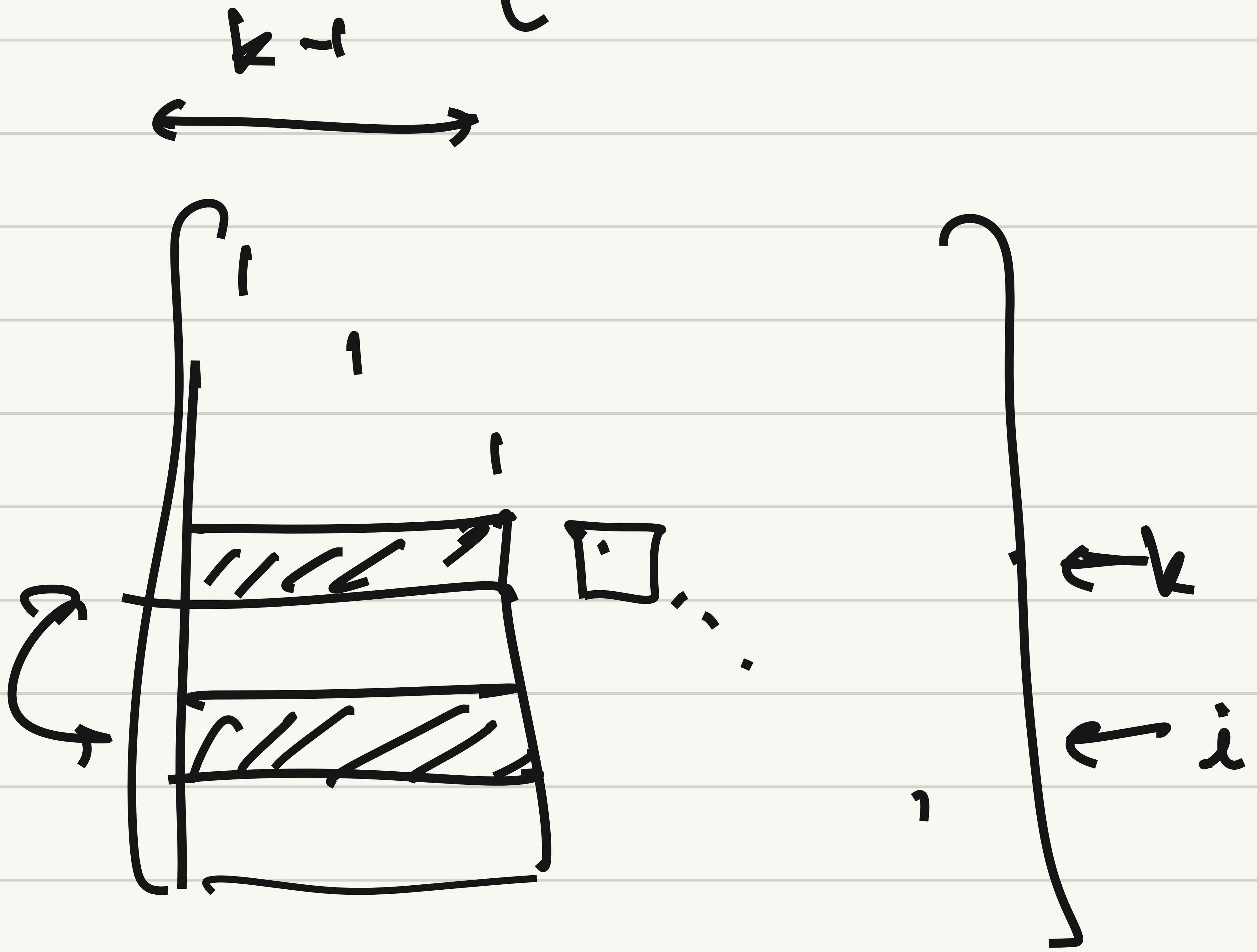
$\hookrightarrow |u_{jk}| / |u_{kk}| \leq 1$

lower tri. matrix with $l_{kk} = 1$

$|l_{jk}| \leq 1$

P_2 : row 2 $\longleftrightarrow$ row i

$$L_1 = \begin{bmatrix} 1 & & & & \\ \boxed{l_{21}} & 1 & & & \\ \vdots & & \ddots & & \\ \boxed{l_{i1}} & & & 1 & \\ \vdots & & & & \ddots \end{bmatrix} \qquad L_1' = \begin{bmatrix} 1 & & & & & \\ \boxed{l_{i1}} & 1 & & & & \\ l_{31} & & 1 & & & \\ \vdots & & & \ddots & & \\ \boxed{l_{21}} & & & & 1 & \\ l_{i+1,1} & & & & & \ddots \\ \vdots & & & & & 1 \end{bmatrix}$$



L

$PA = LU$

Init $L = I$, $U = A$, $P = I$

for each row $k = 1 \dots m-1$

pick best row i to swap with k

swap rows i, k of U, P

swap subdiag. entries of rows i, k of L

for $j = k+1 \dots m$

...

A, b

$QR = \text{house}(A) \longrightarrow O(n^3)$

solve $\underbrace{QR\vec{x} = \vec{b}}_{O(n^2)}$

$L, U, P = \text{lu}(A) \longrightarrow O(n^3)$

solve $\underbrace{LUx = P\vec{b}}_{O(n^2)}$

$PA = LU$

$PAx = LUx$

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

$PA\vec{x} = P\vec{b}$

Householder $\sim \frac{4}{3} m^3$ flops

LU $\sim \frac{2}{3} m^3$ flop