Last time:

<u>Thm</u> (Backward error of GE)

Let $A \in \mathbb{R}^{n\times n}$ and suppose GE produces computed LU factor $\hat{L}$, $\hat{U}$ and a computed solution $\hat{x}$ to $Ax=b$

then $(A+\Delta A)\hat{x} = b$, with $|\Delta A| \le \gamma_{3n} |\hat{L}||\hat{U}|$ $(\star)$

There are two issues regarding GE

Problem 1: $A = LU$ doesn't always exist

$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ but no LU fact. $\leftarrow$ exercise.

Problem 2: $(\star)$ doesn't imply the stability of GE / Doolittle

- $(\star)$ provides a bound $|\Delta A| \le \gamma_{3n} |\hat{L}||\hat{U}|$.

  Ideally, we would like $|\Delta A| \le C_n \varepsilon_{mach} |A|$

  If $|\hat{L}||\hat{U}| = |\hat{L}\hat{U}|$, we obtain that

$$|\hat{L}||\hat{U}| = |\hat{L}\hat{U}| = |A+\Delta A|$$

$$\le |A| + \gamma_n |\hat{L}||\hat{U}|$$

$$\Rightarrow |\hat{L}||\hat{U}| \le \frac{1}{1-\gamma_n}|A|$$

$$\overset{(\star)}{\Rightarrow} |\Delta A| \le \frac{\gamma_{3n}}{1-\gamma_n}|A|$$

- $|\hat{L}||\hat{U}| = |\hat{L}\hat{U}|$ does not always hold true. One condition is that A being totally nonnegative, that is, if the determinant of every square submatrix is nonnegative and ε_{mach} is small enough (to ensure that $\hat{L} \approx L$ and $\hat{U} \approx U$)

- In general, we don't have this condition, and backward error can be quite large.

ex. $A = \begin{bmatrix} \varepsilon & 1 \\ 1 & 1 \end{bmatrix}$, $\quad \kappa_\infty(A) = \frac{4}{1-\varepsilon} \quad (\varepsilon < 1)$

Exact LU fact. $\quad L = \begin{bmatrix} 1 & 0 \\ 1/\varepsilon & 1 \end{bmatrix}$, $\quad U = \begin{bmatrix} \varepsilon & 1 \\ 0 & 1-\frac{1}{\varepsilon} \end{bmatrix}$

If $fl(1 - 1/\varepsilon) = -1/\varepsilon$

$$\hat{L} = \begin{bmatrix} 1 & 0 \\ 1/\varepsilon & 1 \end{bmatrix}, \quad \hat{U} = \begin{bmatrix} \varepsilon & 1 \\ 0 & -1/\varepsilon \end{bmatrix}$$

$$\hat{L}\hat{U} = \begin{bmatrix} \varepsilon & 1 \\ 1 & 0 \end{bmatrix}, \quad |\hat{L}|\,|\hat{U}| = \begin{bmatrix} \varepsilon & 1 \\ 1 & 2/\varepsilon \end{bmatrix}$$

$$A - \hat{L}\hat{U} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad \| |\hat{L}|\,|\hat{U}| \|_\infty = O(\tfrac{1}{\varepsilon})$$

$$\gg \|A\|_\infty = O(1)$$

Def: growth factor

$$\rho_n(A) = \frac{\max\{|L|_\infty, |U|_\infty\}}{|A|_\infty}$$

We should use $|\hat{L}|.\ |\hat{U}|$ but then the definition will involve ε_{mach}, which is cumbersome.

- Goal: Need to control $|L|$ and $|U|$

- Solution: pivoting

At k^{th} stage of GE

$$A^{(k)} = \begin{bmatrix} A_{11}^{(k)} & A_{12}^{(k)} \\ 0 & A_{22}^{(k)} \end{bmatrix} \qquad A_{11}^{(k)} \in \mathbb{R}^{(k-1)\times(k-1)} \text{ upper triangular}$$

$$L = \begin{bmatrix} 1 & & & \\ l_{21} & 1 & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \cdots & 1 \end{bmatrix}, \qquad l_{jk} = \frac{a_{jk}^{(k)}}{a_{kk}^{(k)}}, \quad j = k, \dots, n$$

- Idea: use row permutation to avoid small pivots and control growth in $|L|$

Option 1: Partial pivoting: Select $a_{rk}^{(k)} = \underset{k \le i \le n}{\operatorname{argmax}} |a_{ik}^{(k)}|$ and permute rows

$$\overset{A}{\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \triangle & \times & \times \end{bmatrix}} \xrightarrow{P_1} \overset{P_1 A}{\begin{bmatrix} \triangle & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}} \xrightarrow{E_1} \overset{E_1 P_1 A}{\begin{bmatrix} \triangle & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}}$$

Select pivot

$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

The GE with partial pivoting is equivalent to GE without pivoting applied to row-permuted matrix

ex. $U = E_2 P_2 E_1 P_1 A$

$$= E_2 \cdot P_2 E_1 P_2 \cdot (\underbrace{P_2 P_1}_{P} A) \qquad \text{since } P_i^2 = I$$

$$= \underbrace{E_2 E_i'}_{L^{-1}} PA \quad \Rightarrow \quad PA = LU$$

Let

$E_i = I - l_i e_i^T$

$l_i = (0, \dots, 0, l_{i+1,i}, \dots, l_{ni})^T$

$e_i = (0, \dots, 0, 1, 0, \dots, 0)^T$

↑ ith entry

where $E_i' = P_n \cdots P_{i+1} E_i P_{i+1} \cdots P_n$

$$= I - \underbrace{(P_n \cdots P_{i+1}) l_i}_{=: l_i'} e_i^T$$

From how we choose P_i

$$\max_{k+1 \le j \le n} |l_{jk}'| = \max_{k+1 \le j \le n} |l_{jk}| \overset{\downarrow}{=} \max_{k+1 \le j \le n} \frac{|a_{jk}^{(k)}|}{|a_{kk}^{(k)}|} \le 1.$$

hence $\rho_n(A) = \dfrac{\max\{1, |U|_\infty\}}{|A|_\infty}$

<u>Thm</u> (Wilkinson) Let $A \in \mathbb{R}^{n \times n}$, suppose GE with partial pivoting, and $\hat{x}$ be computed solution $\hat{x}$ to $Ax = b$

then $(A + \Delta A)\hat{x} = b$,

with $\|\Delta A\|_\infty \le n^2 \gamma_{3n} \rho_n(A) \|A\|_\infty$

some constant that polynomially depend on n

Remark: Forward error $\dfrac{\|x - \hat{x}\|}{\|x\|} \lesssim C_n \, \kappa(A) \, \rho_n(A) \, \varepsilon_{mach}$

dependence on n?

• How large is ρ_n?

By induction $|u_{ij}| \le 2^{i-1} \max_{k \le i} |a_{kj}|$ ⟵ exercise

$\Rightarrow \|U\|_\infty \le 2^{n-1} \|A\|_\infty \Rightarrow \rho_n(A) \le 2^{n-1}$ ⟵ exponentially large in n

This bound is achievable:

$$A = \begin{bmatrix} 1 & & & 0 & 1 \\ -1 & 1 & & & 1 \\ -1 & -1 & 1 & & 1 \\ \vdots & \vdots & & \ddots & \vdots \\ -1 & -1 & \cdots & -1 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ -1 & -1 & 1 & & \\ \vdots & \vdots & & \ddots & \\ -1 & -1 & \cdots & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & & 1 \\ & 1 & & & 2 \\ & & 1 & & \vdots \\ 0 & & & \ddots & 2^{n-2} \\ & & & & 2^{n-1} \end{bmatrix}, \quad \rho(A) = 2^{n-1}$$

- $\kappa_\infty(A) = O(n)$

  when $\varepsilon_{mach} = 2^{-53}$, $n = 53$, $\dfrac{\|x - \hat{x}\|}{\|x\|} = O(1)$

  But this not observed in the IJulia notebook on Canvas.

  <u>Why?</u> ⟵ worst-case error

- GE with partial pivoting is NOT backward stable.

  But in practice exponential growth $\rho_n(A)$ seems "rare"

- growth factor for random matrix is small:

  $$\rho_n(A) \approx O(\sqrt{n}) \quad \text{for} \quad a_{ij} \overset{iid}{\sim} N(0,1)$$

Option 2: Complete pivoting: Select $a_{rs}^{(k)} = \underset{k \le i,j \le n}{\operatorname{argmax}} |a_{ij}^{(k)}|$

and permute rows and/or columns

- equivant to apply GE to $\underset{\text{permute rows}}{P} A \underset{\text{permute columns}}{Q} = LU$

- For complete pivoting, $n \le \rho_n(A) \le \frac{1}{2}\sqrt{n}\, n^{\log(n)/4}$

tight bound is open problem

GE is good for dense matrix without structure.

For matrix with structure, GE can be improved.

- Cholesky factorization:

$$A = LL^T \quad , \quad L \text{ low triangular}$$

<u>Thm</u>: If A is symmetric positive definite, then A has a unique Cholesky factorization with positive diagonal elements.

Pf: Since A is positive definite, we know

$\det(A(1:i, 1:i)) > 0, \quad \forall\, i = 1, \dots, n$

This implies $A = LU$ exists ← exercise

Let $U = D\tilde{U}$ where $\tilde{U}$ has unit diagonal element

From symmetricity of A,

$$A^T = A \Rightarrow \underbrace{\tilde{U}^T}_{\text{unit lower triangular}} \overbrace{D^T L^T}^{\text{upper triangular}} = \underbrace{L}_{\text{unit lower triangular}} \overbrace{D\tilde{U}}^{\text{upper triangular}}$$

From uniqueness of LU,

$$\tilde{U}^T = L, \quad D^T L^T = D\tilde{U}$$

So we have $A = LD\tilde{U} = LDL^T$

Clearly $D_{ii} > 0$, Let $\tilde{L} = LD^{1/2}$ then $A = \tilde{L}\tilde{L}^T$

∎

- An algorithm to compute $A = LL^T$ can be derived following how we derive Doolittle's method.

  But operation count $\approx \frac{1}{3}n^3 \leftarrow$ half of GE $(\frac{2}{3}n^3)$

- Similar backward error bound for Cholesky

$$(A + \Delta A)\hat{x} = b, \quad \text{with } |\Delta A| \le \gamma_{3n+1} |\hat{R}|^T |\hat{R}|$$

  But doesn't suffer from growth factor because

$$\| |R|^T |R| \|_2 = \| |R| \|_2^2 \le n \|R\|_2^2 = n \|A\|_2$$

exercise (show that $\| |A| \|_2^2 \le \mathrm{rank}(A) \|A\|_2^2$)

- Nonpositive definite symmetric

$$A = LDL^T$$

- Tridiagonal matrix (Thomas algorithm)

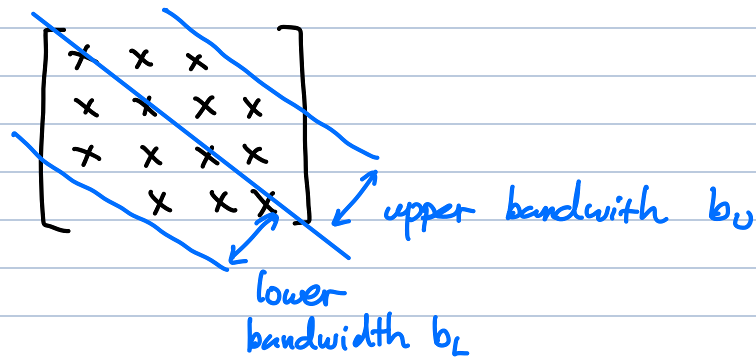
$$A = LU$$

bidiagonal

$$\begin{bmatrix} \times & & & \\ \times & \times & & \\ & \times & \times & \\ & & \times & \times \end{bmatrix}$$

Solve in $O(n)$ FLOPs.

- Banded matrix



$$A = L\ U$$

L: lower triangular with lower bandwidth b_L

U: upper triangular with upper bandwidth b_U

With partial pivoting,

$$PA = L\ U$$

L: lower bandwidth b_L

U: upper bandwidth $b_U + b_L$

Solve in $O(n(b_U+b_L)^2)$

- Sparse matrix : mostly zero entries $\Rightarrow$ sparse direct solvers