Square Linear Systems

Spring 2021 A. Donev

E.g.

$$\begin{cases} 3x_1 + 2x_2 = 2 \\ x_1 - x_2 + x_3 = 1 \\ 2x_1 + 3x_3 = 5 \end{cases}$$

$$\overleftrightarrow{A}\,\vec{x} = \vec{b} \leftarrow \text{r.h.s.}$$

↑ matrix ↖ solution

$$A = \begin{bmatrix} 3 & 2 & 0 \\ 1 & -1 & 1 \\ 2 & 0 & 3 \end{bmatrix} \quad b = \begin{bmatrix} 2 \\ 1 \\ 5 \end{bmatrix}$$

$$A = [m \times n] \quad x = [n \times 1]$$

$$b = [m \times 1]$$

m eqs. , n variables

For a while $\quad m = n$

$$Ax = b \qquad m = n$$

How many solutions?

- 0 → A not invertible, $b \notin \operatorname{Im}(A)$
- 1 → A is invertible
  $x = A^{-1} b$
- ∞ → A not invertible, $b \in \operatorname{Im}(A)$

If A is <u>not</u> invertible.

$Ax = 0$? How many solutions?

Infinitely many solutions

x, αx is also a solution

Back to: $Ax = b$ for non-invertible

$$\begin{cases} Ax_1 = b & \text{has 1 solution} \\ Ax_2 = 0 & \text{- infinitely} \end{cases}$$

$$A(x_1 + x_2) = b$$

$Ax = b$, $b \in im(A)$

If $b \notin im(A) \Rightarrow$ no solution

If $b \in im(A) \Rightarrow$ infin. many solutions

$$Ax = b \quad , A \text{ is invertible}$$

$$\sum_{j=1}^{n} a_{ij} x_j = b_i \quad \forall i \quad i=1,\dots,n$$

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

NOT how we compute it numerically

Never do $x = inv(A) * b$

$$\begin{array}{c c} \rightarrow & \\ -\frac{a_{21}}{a_{11}} & \\ & \end{array}
\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\ a_{21}^{(1)} & a_{22}^{(1)} & a_{23}^{(1)} \\ a_{31}^{(1)} & a_{32}^{(1)} & a_{33}^{(1)} \end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \\ b_3^{(1)} \end{bmatrix}$$

Reduced row echelon form

Step 1: Climmate x_1

a) Multiply 1st equation by

$$l_{21} = \frac{a_{21}}{a_{11}}$$

and subtract it from second equations

b) Multiply 1st equation by

$$l_{31} = \frac{a_{31}}{a_{11}}$$

eq. # → 3, 1 ← var #

and subtract from 3rd eq

$$
\left[\begin{array}{c|c|c}
a_{11} & a_{12} & a_{13} \\
\hline
a_{21} - l_{21} a_{11} = \emptyset & a^{(2)}_{22} = a^{(1)}_{22} - l_{21} \cdot a^{(1)}_{12} & a^{(2)}_{23} = a_{23} - l_{21} \cdot a_{13} \\
\hline
\emptyset & a^{(2)}_{32} = a^{(1)}_{32} - l_{31} a^{(1)}_{12} & a^{(2)}_{33} = a^{(1)}_{33} - l_{31} a^{(1)}_{13}
\end{array}\right]
$$

$$
a^{(k+1)}_{ij} = a^{(k)}_{ij} - l_{ik} \, a^{(k)}_{kj}
$$

$$
\underset{\text{eq.}\uparrow\ \uparrow\text{var}}{l_{ik}} = \frac{a^{(k)}_{ik}}{a^{(k)}_{kk}}, \quad i, j > k
$$

$$
a^{(k)}_{kk} \neq 0
$$

$$\begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \\ b_3^{(1)} \end{bmatrix} \to \begin{bmatrix} b_1^{(2)} = b_1^{(1)} \\ b_2^{(2)} = b_2^{(1)} - l_{21} b_1 \\ b_3^{(2)} = b_3^{(1)} - l_{31} b_1 \end{bmatrix}$$

$$b_i^{(k+1)} = b_i^{(k)} - l_{ik} b_k^{(k)}$$

Step 2

$$\begin{array}{c} \\ l_{21} \\ l_{31} \end{array} \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\ \cancel{0} & a_{22}^{(2)} & a_{23}^{(2)} \\ \cancel{0} & a_{32}^{(2)} & a_{33}^{(2)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \\ b_3^{(2)} \end{bmatrix}$$

Multiply 2^{nd} eq. by

$$\underset{\substack{\uparrow \quad \uparrow \\ \text{eq.} \quad \text{var}}}{l_{32}} = \frac{a_{32}^{(2)}}{a_{22}^{(2)}}$$

and subtract from 3^{rd} eq.

$$\begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\ l_{21}\,\cancel{0} & a_{22}^{(2)} & a_{23}^{(2)} \\ l_{31}\,\cancel{0} & l_{32}\,\cancel{0} & a_{33}^{(3)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(2)} \\ b_3^{(3)} \end{bmatrix}$$

<u>Step 3</u>:

$$x_3 = \frac{b_3^{(3)}}{a_{33}^{(3)}}$$

Step 4:

$$x_2 = \frac{b_2^{(2)} - a_{23}^{(2)} x_3}{a_{22}^{(2)}}$$

Step 5: solve for x_1

Gaussian elimination

$$L = \begin{bmatrix} 1 & \emptyset & \emptyset \\ l_{21} & 1 & \emptyset \\ l_{31} & l_{32} & 1 \end{bmatrix}$$

$\det(L)=1$ is invertible

unit lower triangular matrix

$$U = \begin{bmatrix} a_{11}^{(1)} & a_{12}^{(1)} & a_{13}^{(1)} \\ \emptyset & a_{22}^{(2)} & a_{23}^{(2)} \\ \emptyset & \emptyset & a_{33}^{(3)} \end{bmatrix}$$

upper triangular

<u>Theorem</u>: $A = LU$

LU factorization

$\Longleftrightarrow$ Gauss elimination

Code MyLU.m on webpage

$i > k$: $l_{ik} = \dfrac{a_{ik}}{a_{kk}} \Rightarrow a_{ik}$

$l_{kk} = 1$ (not stored)

for $k = 1 : (n-1)$

Eliminate x_k from eqs. $k+1, \dots, n$

$A((k+1):n, k) =$

$A((k+1):n, k) / A(k,k);$

Compute $l_{ik}, i > k$

$$a_{ij} \Leftarrow a_{ij} - l_{ik} a_{kj}$$

$$i, j > k$$

for $j = (k+1) : n$

$A((k+1):n, j) = A((k+1):n, j)$

$- \underbrace{A((k+1):n, k)}_{\text{stores } l_{ik}} * A(k, j);$

"in-place"
LU
factorization

end [for j]

end [for k]

Note We could have done
for $i = (k+1) : n$

Last time: $Ax = b$

GEM: $A = L\,U$

lower (L), upper triang. (U)

"Proof": $\Updownarrow$

$$a_{ij} = \sum_{k=1}^{n} l_{ik}\, u_{kj}$$

Dot product between i'th row of L and j^{th} column of U

$$a_{ij} = \sum_{k=1}^{\min\{i,j\}} l_{ik}\, u_{kj}$$

If $i > j \Rightarrow \sum_{k=1}^{j}$

If $i \leq j \Rightarrow \sum_{k=1}^{i}$

Recall $l_{ii} = 1$

(1) $$a_{ij} = \sum_{k=1}^{i} l_{ik} u_{kj}$$

$i = 1, \dots, n$

$j = i, \dots, n$

$l_{ii} = 1$

$$= \sum_{k=1}^{i-1} l_{ik} u_{kj} + u_{ij}$$

$$\Rightarrow u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$

✓ GEM

We need $l_{i,(k<i)}$

$u_{(k<i),j}$

$$a_{ij}^{(k+1)} = a_{ij}^{(k)} - l_{ik} \cdot a_{kj}^{(k)}$$

(2) $$a_{ij} = \sum_{k=1}^{j} l_{ik} u_{kj}$$

$$i > j$$

$$l_{ij} = \frac{\left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj}\right)}{u_{jj}}$$

$$l_{ij} = \frac{a_{ij}^{(j)}}{a_{jj}^{(j)}}$$

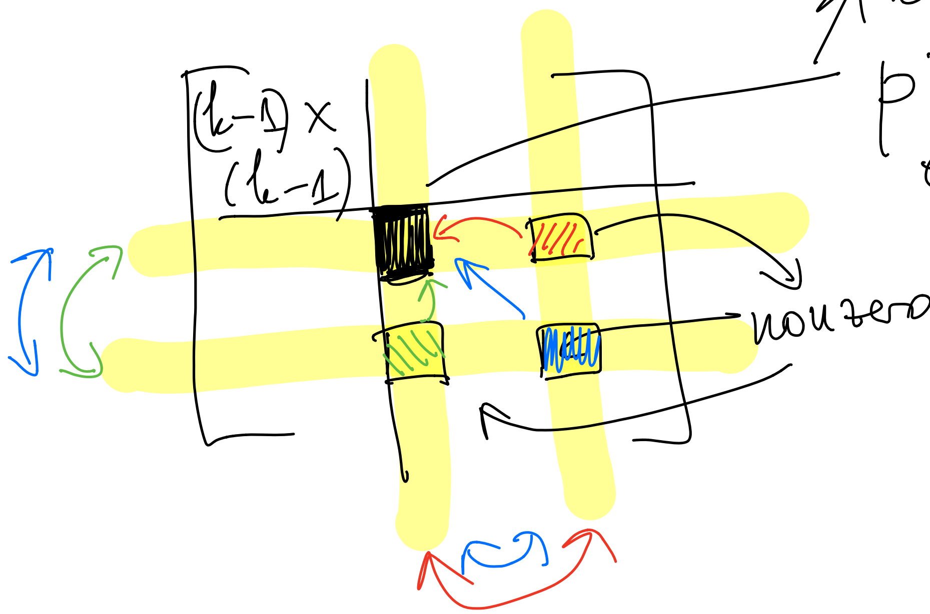
Which shows that GEM computed L & U s.t.

$$A = LU$$

Pivoting

Assumed that $a_{kk}^{(k)} \neq 0$

pivot element



Pivoting: Row, Column, Complete = row + column

Let's re-order equations

$$
\begin{array}{r}
2\times \\
3\times
\end{array}
\begin{bmatrix} 1 & 1 & 3 \\ 2 & 2 & 2 \\ 3 & 6 & 4 \end{bmatrix}
\begin{bmatrix} x_1 = 1 \\ x_2 = 1 \\ x_3 = 1 \end{bmatrix}
=
\begin{bmatrix} 5 \\ 6 \\ 13 \end{bmatrix}
$$

$$\Downarrow$$

$$
\begin{bmatrix} 1 & 1 & 3 \\ 0 & \boxed{0} & -4 \\ 0 & 3 & -5 \end{bmatrix}
\Rightarrow
\begin{bmatrix} 5 \\ -4 \\ -2 \end{bmatrix}
$$

$$
\begin{bmatrix} 1 & 1 & 3 \\ 0 & 3 & -5 \\ 0 & 0 & -4 \end{bmatrix}
\begin{bmatrix} x_1 = 1 \\ x_2 = 1 \\ x_3 = 1 \end{bmatrix}
=
\begin{bmatrix} 5 \\ -2 \\ -4 \end{bmatrix}
$$

$$
L = \begin{bmatrix} 1 & & \\ 2 & 1 & 1 \\ 3 & 0 & \end{bmatrix}
$$

$$
LU = \underset{\uparrow}{P} A
$$

permutation matrix

Theorem:

If A is non-singular then pivoted LU factorization will succeed

$$PA = LU$$

for some permutation matrix P

What is the best P

Example:

$$\left[\begin{array}{c|c} 10^{-20} & 1 \\ \hline 1 & 1 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$$x_1 \simeq x_2 \simeq 1$$

$$\|$$

$\Downarrow$ GEM

$10^{20} \times$

$$\left[\begin{array}{c|c} 10^{-20} & 1 \\ \hline \cancel{0} & 1-10^{20} \end{array}\right]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2-10^{20} \end{bmatrix}$$

Due to roundoff

$$\left[\begin{array}{c|c} 10^{-20} & 1 \\ \hline & -10^{20} \end{array}\right]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -10^{20} \end{bmatrix}$$

$$x_2 = \frac{-10^{20}}{-10^{20}} = \underline{1} \quad \checkmark$$

$$10^{-20} x_{\underline{1}} = \underline{1} - \underline{1} = 0$$

$$\Rightarrow \quad x_{\underline{1}} = 0 \neq \underline{1} \quad \times$$

Not the correct solution

$$\begin{bmatrix} 1 & 1 \\ 10^{-20} \approx 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

$$x_1 = x_2 = \underline{1} \quad \checkmark$$

Or change order of variables

$$\begin{bmatrix} 1 & 10^{-20} \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_2 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

"Small" pivot elements are a problem in floating-point arithmetic

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}$$

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

$$\Downarrow$$

$$\begin{bmatrix} 7 & 8 & 0 \\ 0 & 3/7 & 6 \\ 0 & 6/7 & 3 \end{bmatrix} \begin{bmatrix} \\ \\ \\ \end{bmatrix} = \begin{bmatrix} 2 \\ -8/7 \\ 5/7 \end{bmatrix}$$

$$\to \begin{bmatrix} 7 & 8 & 0 \\ 0 & 6/7 & 3 \\ 0 & 3/7 & 6 \end{bmatrix} \cdots \begin{bmatrix} 2 \\ 5/7 \\ -8/7 \end{bmatrix}$$

$$\Downarrow$$

$$\begin{bmatrix} 7 & 8 & 0 \\ 0 & 6/7 & 3 \\ 0 & 0 & 9/2 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 5/7 \\ -3/2 \end{bmatrix}$$

$$P^{-1} \;\Big|\; PA = LU = Pb$$

$$P^{-1} = P^T$$

$$A = P^T L U = b$$

$$A = (P^T L)\, U = \tilde{L}\, U$$

$$
\begin{array}{c}1\\2\\3\end{array}
\begin{bmatrix} D & & \\ D & D & \\ D & D & D \end{bmatrix}
\qquad
\begin{array}{c}3\\2\\1\end{array}
\begin{bmatrix} D & D & D \\ D & D & \\ D & & \end{bmatrix}
$$

permuted lower triangel

In MATLAB:

$$Ax = b$$

$$A = LU$$

$$L(\underbrace{Ux}_{=y}) = b$$

(1) $Ly = b$ to get y — forward subst.

(2) $Ux = y$ for x — backward substitution

$$\begin{bmatrix} l_{11} & & & \\ l_{21} & l_{22} & & \\ \vdots & \vdots & & \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \end{bmatrix}$$

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

$$y_1 = b_1 / l_{11}^{=1} = b_1$$

$$y_2 = \frac{b_2 - l_{11} y_1}{l_{22} = 1}$$

$$Ly = b$$

$$y_i = \frac{b_i - \sum_{j=1}^{i-1} l_{ij} y_j}{l_{ii} = 1}$$

$$i = 1, \dots, n$$

Matlab code

Forward substitution

```
for i = 1 : n
y(i) = b(i) - sum(L(i,1:i-1).*
                 y(1:i-1))
end
```

For $Ux = y$ (Backward)

```
for i = n : -1 : 1
```

Homework

Matlab syntax

"mldivide"

```
[L, U, P] = lu(A)
```

L is really $\tilde{L}$

```
y = L̃ \ b;   % Solve Ly=b
x = U \ y;   % Solve Ux=y
```

alent

equiv.

To solve $A*x = b$ in Matlab

$$x = A \backslash b;$$ "mldivide"

Different from $x = \text{inv}(A)*b$

never do this

Equivalent:

P is hidden

$$x = \underline{U} \backslash (\underline{L \backslash b});$$

important

Things we care about:

→ Convergence (?)
(consistent, stable)

→ Speed of convergence
(order of accuracy)

→ Robustness

opposition

→ Roundoff error (stability, error propagation) (Backward stability)

→ Efficiency (computational complexity)

Complexity of LU fact.

FLOPS = floating point operations

+, −, *, /

Backward / forward substitution

for $i = 1 : n$

$y(i) = b(i) - \text{sum}\big(L(i, 1:i-1)$

$.* \; y(1:i-1)\big)$

end

$L(i, 1:i-1) \cdot y(1:i-1)$

dot product

$i-1$ multiplications (elementwise)

$\underbrace{1 + i - 2}$ additions

$2*(i-1)$ FLOPS

$$2 \sum_{i=1}^{n} (i-1) = \cancel{2}\frac{n(n-1)}{\cancel{2}}$$

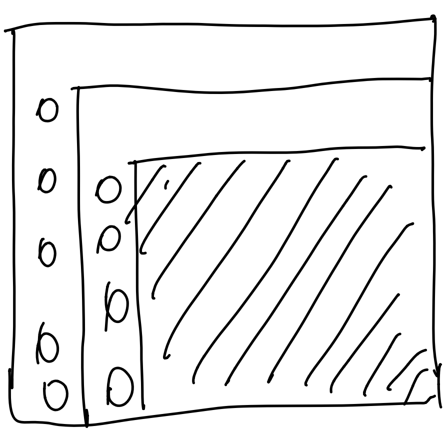
$0 \quad 1 \quad 2 \quad \dots \quad (n-3) \quad (n-2) \quad (n-1)$

$n-1$

$$\# \text{FLOPS} = n(n-1) \approx n^2 - \underbrace{\cancel{n}}_{\text{small}}$$

Forward / backward subst.
takes $\sim n^2$ FLOPS
$O(n^2)$ operations

LU factorization cost



n

$n-1$

$\dots$

$(n-k+1)\times(n-k+1)$

$\Downarrow$

$(n-k)\times(n-k)$

Step k takes $O((n-k)^2)$ FLOPs (coefficient in worksheet 3)

$$\sum_{k=1}^{n-1} (n-k)^2 = \sum_{k=1}^{n-1} k^2$$

$$= \begin{cases} \int_{k=1}^{n} k^2 \, dk \sim \frac{n^3}{3} \\ a_3 n^3 + a_2 n^2 + a_1 n + a_2 \end{cases}$$

correct leading-order term

LU factorization takes $O(n^3)$ FLOPs $\gg O(n^2)$

All matrix factorizations

$\sim O(n^3)$

Stability of problems

$$Ax = b$$

$$(A+\delta A)(x+\delta x) = b + \delta b$$

$$\frac{\|\delta A\|}{\|A\|} \geq 10^{-16} \qquad \frac{\|\delta b\|}{\|b\|} \geq 10^{-16}$$

Question $\frac{\|\delta x\|}{\|x\|} = ?$

$$\frac{\|\delta x\|}{\|x\|} \leq K(A) \frac{\|\delta b\|}{\|b\|}$$

conditioning number

$$K(A) = \|A\| \|A^{-1}\|$$

(depends on choice of norm)

$$x \longrightarrow Ax$$

$$x + \delta x \xrightarrow{K(A)} Ax + ?$$

relative change

e.g. $K(A) \approx 10^4$

6 digits in x $\rightarrow$ $6-4=2$ digits in Ax

Our case

$$x \longrightarrow A^{-1}b$$

$$b \longrightarrow A^{-1}b$$

$$K(A^{-1}) = \|A^{-1}\| \|(A^{-1})^{-1}\|$$

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

$$\kappa(A^{-1}) = \kappa(A)$$

$$\frac{\|\delta x\|}{\|x\|} \geq \underset{\underset{10^{-16}}{\wr\wr}}{\varepsilon} \cdot \kappa(A)$$

$\kappa(A) = 10^{p}$ means loose p digits

$p \gg 1$ ill-conditioned matrix / system

Most of the time, pivoted LU factorization gives us this accuracy (does not loose extra digits)

$$Ax = b$$

$$\|Ax - b\| = 0$$

$$r = Ax - b$$

$$\boxed{\text{Always check solution by computing } \|r\| = \|Ax - b\|}$$

$$\frac{\|r\|}{\|b\|} \sim 10^{-16}$$

We really want this backwards stability.

"Theorem": Pivoted LU is backwards stable

More precisely:

$$x = A \backslash b$$

$$(A + \delta A)\, x = b + \delta b$$

$$\frac{\|\delta A\|}{\|A\|} \sim \frac{\|\delta b\|}{\|b\|} \sim 10^{-16}$$