CSC338 Lecture 4

Last time: $A\underline{x} = \underline{b}$ for $A \in \mathbb{R}^{n \times n}$ nonsingular

Use Gauss Elimination and LU Factorization

Question: when does Gauss Elimination fail?

eg// ① $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 2 & 2 \end{bmatrix}$

This element, called the pivot is zero!

$R_4 \leftarrow R_4 - \frac{2}{0} R_3$ we can't divide by 0!

eg// ② $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 0.0001 & 2 \\ 0 & 0 & 2 & 2 \end{bmatrix}$

This pivot is close to zero

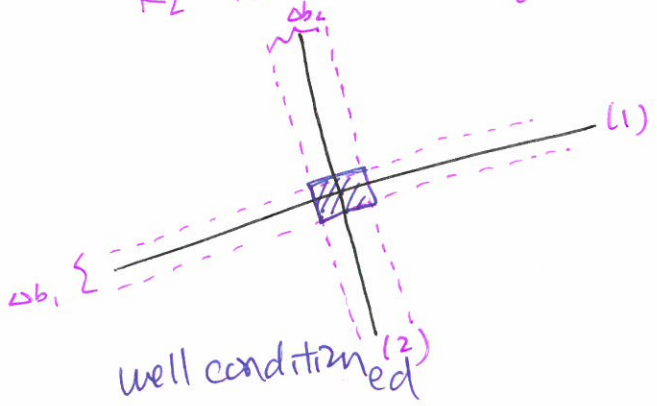
$R_4 \leftarrow R_4 - \underbrace{\frac{2}{0.0001}}_{\text{very large}} R_3$

Examples ① and ② points to issues with the stability of the algorithm

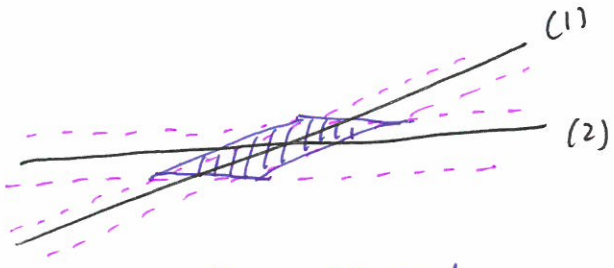
eg// $A = \begin{bmatrix} 4.11 & 5.0 \\ 8.23 & 10.1 \end{bmatrix}$ $\underline{b} = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$ $\overset{G.E.}{\Rightarrow}$ $\underline{x} = \begin{bmatrix} 0.487 \\ 0 \end{bmatrix}$ $A\underline{x} = \begin{bmatrix} 2 \\ 4.005 \end{bmatrix}$

This matrix is "almost singular"

R_2 is almost equal to $2 \times R_1$



well conditioned



ill conditioned system

(1) $-a_{11}x_1 + a_{12}x_2 = b_1 + \Delta b_1$

(2) $-a_{12}x_1 + a_{22}x_2 = b_2 + \Delta b_2$

eg// $A = \begin{bmatrix} 0.780 & 0.563 \\ 0.913 & 0.659 \end{bmatrix}$ $\underline{b} = \begin{bmatrix} 0.217 \\ 0.254 \end{bmatrix}$

we obtained 2 solutions computationally:

$\hat{\underline{x}}_1 = \begin{bmatrix} 0.341 \\ -0.087 \end{bmatrix}$ $\hat{\underline{x}}_2 \begin{bmatrix} 0.999 \\ -1.001 \end{bmatrix}$

which solution is better?

$\underline{r}_1 = \underline{b} - A\hat{\underline{x}}_1 = \begin{bmatrix} +0.000001 \\ 0 \end{bmatrix}$

$\underline{r}_2 = \underline{b} - A\hat{\underline{x}}_2 = \begin{bmatrix} 0.001343 \\ 0.000572 \end{bmatrix}$

but $\underline{x}^* = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

$\Rightarrow$ Residuals not always a good indicator of accuracy

(Linearly scaling A, $\underline{b}$ will affect $\|\underline{r}\|$ but not $\|\underline{x}^* - \hat{\underline{x}}\|$)

To be able to discuss conditioning/stability, we need a way to talk about the "size" of a vector/matrix.

Def A vector norm $\|\cdot\|$ is a mapping $\mathbb{R}^n \to \mathbb{R}^{\geq 0}$ such that:

1. $\forall \underline{x} \in \mathbb{R}^n$, $\|\underline{x}\| \geq 0$ with $\|\underline{x}\| = 0$ iff $\underline{x} = \underline{0}$
2. $\forall \underline{x} \in \mathbb{R}^n$, $c \in \mathbb{R}$ $\quad \|c\underline{x}\| = |c| \cdot \|\underline{x}\|$
3. $\forall \underline{x}, \underline{y} \in \mathbb{R}^n$ $\quad \|x+y\| \leq \|x\| + \|y\|$.

(triangle inequality)

In this course, we will use the p-norm.

$$\|\underline{x}\|_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}$$

eg// 1-norm $p=1$ $\quad \|\underline{x}\|_1 = \sum_{i=1}^{n} |x_i|$

2-norm $p=2$ $\quad \|\underline{x}\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2}$ ~ Euclidean Norm

∞-norm $p=\infty$ $\quad \|\underline{x}\|_\infty = \max_{1 \leq i \leq n} |x_i|$

eg// $\underline{x} = \begin{bmatrix} 2 \\ 3 \\ -4 \\ 1 \end{bmatrix}$

$\|\underline{x}\|_1 = 10$

$\|\underline{x}\|_2 = \sqrt{4+9+16+1} = \dots$

$\|\underline{x}\|_\infty = 4.$

Def An induced matrix norm is a matrix norm defined in terms of a vector norm as follows:

$$\|A\| \overset{\text{def}}{=} \max_{\|\underline{x}\|=1} \|A\underline{x}\| = \max_{\underline{x}\neq 0} \frac{\|A\underline{x}\|}{\|\underline{x}\|}$$

$\|A\|$: matrix norm

$\|A\underline{x}\|$: vector norm

$\|\underline{x}\|$: vector norm

The largest possible value of $\|A\underline{x}\|$ across all possible vectors $\underline{x}$ where $\|\underline{x}\| = 1$.

Properties of Matrix Norms

1. $\|A\| \geq 0$ with $\|A\| = 0$ iff $A = 0$ ← the zero matrix.
2. $\|cA\| = |c|\|A\|$ for $c \in \mathbb{R}$
3. $\|A+B\| \leq \|A\| + \|B\|$
4. $\|AB\| \leq \|A\|\|B\|$
5. $\|A\underline{x}\| \leq \|A\|\|\underline{x}\|$
6. $\|I\| = 1$

~~eg//~~

we can also show: $\|A\|_1 = \max_j \sum_{i=1}^{m} |a_{ij}|$ ~ max abs column sum

$\|A\|_\infty = \max_i \sum_{j=1}^{n} |a_{ij}|$ ~ max abs. row sum.

eg// $A = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}$

$\|A\|_1 = 4$

$\|A\|_\infty = 4$

$\|A\| = 4$

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

$\|A\|_1 = 5$

$\|A\|_\infty = 4$

Def The condition number of an $n \times n$ matrix A is defined to be

$$\text{cond}(A) = \begin{cases} \|A\| \cdot \|A^{-1}\| & \text{if } A \text{ is nonsingular} \\ \infty & \text{if } A \text{ is singular} \end{cases}$$

we can show that

$$\|A\| \|A^{-1}\| = \left(\max_{\|\underline{x}\|=1} \|A\underline{x}\| \right) \left(\min_{\|\underline{x}\|=1} \|A\underline{x}\| \right)^{-1}$$

max stretch — max shrink

$\Rightarrow$ cond(A) describes the ratio of the max stretch to max shrinking of unit vectors

Properties of cond(A)

1. $\text{cond}(A) = \|A\| \cdot \|A^{-1}\| \geq \|A \cdot A^{-1}\| = \|I\| = 1$

   $\text{cond}(A) \geq 1$

2. $\text{cond}(I) = 1$.

3. For $\gamma \in \mathbb{R}$, $\gamma \neq 0$

   $\text{cond}(\gamma A) = \|\gamma A\| \cdot \|\frac{1}{\gamma} A^{-1}\| = \text{cond}(A)$

Claim If cond(A) is small, then $A\underline{x} = \underline{b}$ is well-conditioned.

(small perturbations in A and $\underline{b}$ will not cause large perturbation in the computed solution ~~for~~ $\underline{x}$).

Specifically, we have

$$\frac{\|\Delta \underline{x}\|}{\|\underline{x}^*\|} \leq \text{cond}(A) \frac{\|\Delta \underline{b}\|}{\|\underline{b}\|}, \qquad \frac{\|\Delta \underline{x}\|}{\|\underline{x}^*\|} \leq \text{cond}(A) \frac{\|\Delta A\|}{\|A\|}$$

we will show this — in the textbook.

(Resume 4:10)

Why did we define $\text{cond}(A) = \|A\| \cdot \|A^{-1}\|$?

Recall the definition of C.N. from lecture 1.

$$\text{C.N.} = \frac{|\Delta y / y|}{|\Delta x / x|} \quad \text{or} \quad \underbrace{\left|\frac{\Delta y}{y}\right|}_{\text{relative error of output.}} = \text{C.N.} \underbrace{\left|\frac{\Delta x}{x}\right|}_{\text{relative error of input (problem)}}$$

Pf (that $\frac{\|\Delta \underline{x}\|}{\|\underline{x}^*\|} \le \text{cond}(A) \frac{\|\Delta \underline{b}\|}{\|\underline{b}\|}$)

Consider $A\underline{x} = \underline{b}$.

Let $\underline{x}^*$ be the true solution $\quad A\underline{x}^* = \underline{b}$ — (1)

$\hat{\underline{x}}$ be the computed solution $\quad A\hat{\underline{x}} = \underline{b} + \Delta\underline{b}$ — (2)

$$\Delta \underline{x} = \hat{\underline{x}} - \underline{x}^*$$

from (2) — $A\hat{\underline{x}} - \underline{b} = \Delta \underline{b}$

from (1) — $A\underline{x}^* - \underline{b} = \underline{0}$

Subtract $A(\hat{\underline{x}} - \underline{x}^*) = \Delta \underline{b}$ So $A\,\Delta \underline{x} = \Delta \underline{b}$

So we have $\Delta \underline{x} = A^{-1} \Delta \underline{b} \Rightarrow \|\Delta \underline{x}\| \le \|A^{-1}\| \cdot \|\Delta \underline{b}\|$. — (3)

$A\underline{x}^* = \underline{b} \Rightarrow \|A\| \cdot \|\underline{x}^*\| \ge \|\underline{b}\|$ — (4)

(3)/(4)

$$\frac{\|\Delta \underline{x}\|}{\|A\|\,\|\underline{x}^*\|} \le \frac{\|A^{-1}\|\,\|\Delta \underline{b}\|}{\|\underline{b}\|}$$

Norm relative error of the computed solution $\left\{ \frac{\|\Delta \underline{x}\|}{\|\underline{x}^*\|} \le \underbrace{\|A\| \cdot \|A^{-1}\|}_{\text{cond}(A)} \frac{\|\Delta \underline{b}\|}{\|\underline{b}\|} \right\}$ Norm residual of computed solution

Conclusion If cond(A) is small } property of the problem
and relative residual is small } property of the computed solution
then the relative error is small.

But if Δb is small but cond(A) large,
the relative error could still be large.

Improving the Stability of Gauss Elimination

eg// $\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$ $\begin{bmatrix} 0.0001 & 1 \\ 1 & 1 \end{bmatrix}$

↑ can't divide by 0

↑ multiplication by a large number increase error

Idea: Interchange rows $(R_1 \leftrightarrow R_2)$ before eliminating elements below a diagonal, so we maximize the absolute value of the pivot. ~ the value in the diagonal

eg// $A = \begin{bmatrix} 3 & 2 & 9 \\ 4 & 5 & 1 \\ 5 & 2 & 3 \end{bmatrix}$ $R_1 \leftarrow R_3$ since $|-5|$ has the largest abs val in the first column.

We can use a permutation matrix to express the interchange.

$R_1 \leftrightarrow R_3 \Rightarrow P_1 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$ $P_1 A = \begin{bmatrix} -5 & 2 & 3 \\ 4 & 5 & 1 \\ 3 & 2 & 9 \end{bmatrix}$.

Def A permutation matrix P has exactly one 1 in each row and each column, and 0 everywhere else.

Properties.

1. $P^{-1} = P^T$
2. cond(P) = 1.
3. Multiplying by both sides of $A\underline{x} = \underline{b}$ by P does not change the solution $PA\underline{x} = P\underline{b}$

Gauss Elimination with Partial Pivoting

Before eliminating below a diagonal, permute the matrix A so that the pivot ~~has~~ is the largest ~~magnitude~~ element at or below the diagonal.

Instead of performing

$$M_{n-1} \cdots M_2 M_1 A = U$$

M_i = elementary matrix

we perform

$$M_{n-1} P_{n-1} \cdots M_2 P_2 M_1 P_1 A = U$$

where P_i = permutation matrix

It turns out that the above can be expressed as:

$$\underbrace{(\hat{M}_{n-1} \cdots \hat{M}_2 \hat{M}_1)}_{\text{lower triangular } L^{-1}} \underbrace{(P_{n-1} \cdots P_2 P_1)}_{\text{permutation matrix } P} A = U \Rightarrow PA = LU$$

Summary To solve $Ax = b$

1. Find P, L, U s.t. $PA = LU$ using G.E + partial pivoting.
2. To solve $Ax = b \iff PAx = Pb$
   $\iff LUx = Pb$

   Solve $Ly = Pb$ for y

   $Ux = y$ for x.

eg// $A = \begin{bmatrix} \epsilon & 1 \\ 1 & 1 \end{bmatrix}$ with $\epsilon < \epsilon_{mach}$

To eliminate a_{11}
$R_2 \leftarrow R_2 - \frac{1}{\epsilon} R_1$

without pivoting we get

$$L = \begin{bmatrix} 1 & 0 \\ \frac{1}{\epsilon} & 1 \end{bmatrix} \quad U = \begin{bmatrix} \epsilon & 1 \\ 0 & 1 - \frac{1}{\epsilon} \end{bmatrix} \overset{\text{float}}{=} \begin{bmatrix} \epsilon & 1 \\ 0 & -\frac{1}{\epsilon} \end{bmatrix}$$

$$\Rightarrow LU = \begin{bmatrix} 1 & 0 \\ 1/\epsilon & 1 \end{bmatrix} \begin{bmatrix} \epsilon & 1 \\ 0 & -1/\epsilon \end{bmatrix} = \begin{bmatrix} \epsilon & 1 \\ 1 & 0 \end{bmatrix} \neq A$$

Complete Pivoting

In complete pivoting (full pivoting) we search for the largest entry in the remaining submatrix.

eg//

$$\begin{bmatrix} 1 & 2 & 5 & 9 \\ 0 & 3 & -1 & 2 \\ 0 & 4 & 2 & 1 \\ 0 & -1 & -5 & 0 \end{bmatrix}$$

Partial pivoting: $R_2 \leftrightarrow R_3$ Pivot = 4.

Full Pivoting $R_2 \leftrightarrow R_4$ Pivot = -5
$C_2 \leftrightarrow C_3$

Full pivoting changes the solution of the system, but predictably

eg//

$$\begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 2 \\ 3 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$x_1 = 1/2$
$x_2 = 1/3$
$x_1 = 1/3$
$x_2 = 1/2$

we need to keep track of the column swaps.

In practice, full pivoting is expensive, and partial pivoting provides good enough stability.

eg// $A = \begin{bmatrix} 1 & 2 \\ k & 1 \end{bmatrix}$. $k \in [0, 2]$ $A^{-1} = \frac{1}{1-2k}\begin{bmatrix} 1 & -k \\ -2 & 1 \end{bmatrix}$

What would k have to be for $\text{cond}(A)$ to be large.

Use $\|\cdot\|_1$, we have

$$\text{cond}(A) = \|A\|_1 \cdot \|A^{-1}\|_1$$

$$= 3 \cdot \frac{1}{1-2k} \cdot 3$$

which is large when $k \to 0.5$