MATH 125 Lecture 17 and 18 Gaussian Elimination

LU decomposition

The simplest linear system

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 20 \\ -10 \end{bmatrix}$$

$x_1 = 4$ $\quad x_2 = 40$ $\quad x_3 = \frac{10}{3}$

In general, consider $Dx = b$; D is a diagonal matrix with non-zero entries on diagonal $\Rightarrow x_i = \frac{b_i}{d_{ii}}$ $\quad 1 \le i \le n$

The next simplest linear system is:

$Rx = b$ $\quad R \in \mathbb{R}^{n \times n}$; $b \in \mathbb{R}^n$; $x \in \mathbb{R}^n$

$$R = \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1n} \\ & r_{22} & r_{23} & \cdots & r_{2n} \\ & & \ddots & & \vdots \\ & 0 & & \ddots & \vdots \\ & & & & r_{nn} \end{bmatrix}$$

claim The system has a unique solution if $r_{ii} \neq 0$ for $1 \le i \le n$

proof. $\det(R) = r_{11} r_{22} \cdots r_{nn}$ (A fact from linear algebra)

$\therefore r_{ii} \neq 0$ for $1 \le i \le n$

Solving $Rx = b$ $\quad \cdot \; r_{nn} x_n = b_n$ $\quad x_n = \frac{b_n}{r_{nn}}$

$\cdot \; r_{n-1,n-1} x_{n-1} + r_{n-1,n} x_n = b_{n-1}$ (we already know x_n)

$$x_{n-1} = \frac{b_{n-1} - r_{n-1,n} x_n}{r_{n-1,n-1}}$$

proceed to compute $x_{n-2}, x_{n-3}, \ldots, x_1$

Algorithm $\quad x_i = \frac{1}{r_{ii}} \left(b_i - \sum_{j=i+1}^{n} r_{ij} x_j \right)$ $\quad i = n-1, n-2, \ldots, 1$

* This is called back substitution or backward substitution.

Algorithm $\quad$ Input : $R \in \mathbb{R}^{n \times n}$; $b \in \mathbb{R}^n$

output : $x \in \mathbb{R}^n$ such that $Rx = b$

Pseudo code

```
x_n = b_n / r_nn
for i = n-1 : 1
    x_i = b_i
    for j = i+1 : n
        x_i = x_i - r_ij x_j
    x_i = x_i / r_ii
```

Theorem The system $Rx = b$ can be solved using back substitution in $O(n^2)$ time

proof

$$\sum_{i=1}^{n-1}\left[1 + \sum_{j=i+1}^{n} 2\right]$$

$$= \sum_{i=1}^{n-1} 1 + \sum_{i=1}^{n-1}\left(\sum_{j=i+1}^{n} 2\right)$$

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

$$= (n-1) + 2\sum_{i=1}^{n-1}(n-1) + 2\sum_{i=1}^{n} i \qquad \text{Recall } \sum_{i=1}^{n} i = \frac{n(n+1)}{2}$$

$$= (n-1) + 2n(n-1) - 2\frac{(n-1)(n)}{2}$$

$$= (n-1) + 2n^2 - 2n - n^2 + n = n^2 - 1$$

Add the cost of $x_n = b_n / r_{nn} \Rightarrow 1$ flop $\quad n^2 - 1 + 1 = n^2$

Exactly n^2 time

Remark : Let $\tilde{x}$ be the computed solution of $Rx = b$

Then $(R + \Delta R)\tilde{x} = b$ with $\Delta R \in \mathbb{R}^{n\times n}$ satisfying

$$\frac{\|\Delta R\|}{\|R\|} = O(\varepsilon_{machine})$$

Back substitution is backward stable

Proof not trivial! [Easier version will be homework]

We want to solve the system $Ax = b$ with

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & & & \\ a_{m1} & & & a_{mm} \end{bmatrix} \in \mathbb{R}^{m\times m} \qquad b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

Example $A = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} \qquad b = \begin{bmatrix} 1/2 \\ 0 \\ -2 \\ 7 \end{bmatrix} \Rightarrow$ For simplicity $b = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$

step 1 Eliminate x_1 from 2^{nd}, 3^{rd} and 4^{th} equations

Second equation $- \frac{a_{21}}{a_{11}} \cdot$ first equation

Third equation $- \frac{a_{31}}{a_{11}} \cdot$ first equation

Fourth equation $- \frac{a_{41}}{a_{11}} \cdot$ first equation

Notation $\quad l_{21} = \dfrac{a_{21}}{a_{11}} = 2 \qquad l_{41} = \dfrac{a_{41}}{a_{11}} = 3$

$l_{31} = \dfrac{a_{31}}{a_{11}} = 4$

$$\tilde{A} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 3 & 5 & 5 \\ 0 & 4 & 6 & 8 \end{bmatrix} \qquad \tilde{b} = \begin{bmatrix} b_1 \\ b_2 - 2b_1 \\ b_3 - 4b_1 \\ b_4 - 3b_1 \end{bmatrix} \qquad \tilde{b} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Could this action be represented by matrix multiplication?

$$L_{21} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad L_{21} A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$$

$$= \begin{bmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$$

$$L_{21} b = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 - 2b_1 \\ b_3 \\ b_4 \end{bmatrix}$$

Similarly $\quad L_{31} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad L_{41} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{bmatrix}$

Therefore, step 1 is equivalent to:

$$\tilde{A} = L_{41} L_{31} L_{21} A$$
$$\tilde{B} = L_{41} L_{31} L_{21} b$$

(For convenience, drop tildes $(\tilde{A} \ \tilde{b}) \longrightarrow (A \ b)$)

Step 2 $\quad$ Eliminate x_2 from 2^{rd} and 4^{th} equation

Third ~~second~~ equation $- \dfrac{a_{32}}{a_{22}} \cdot$ second equation

Fourth equation $- \dfrac{a_{42}}{a_{22}} \cdot$ second equation

$l_{32} = 3 \quad l_{42} = 4 \qquad \tilde{A} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 2 & 4 \end{bmatrix} \qquad \tilde{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 - 3b_2 \\ b_4 - 4b_2 \end{bmatrix}$

$$L_{32} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -3 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad L_{42} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -4 \end{bmatrix}$$

$$\tilde{A} = L_{32} L_{42} L_{41} L_{31} L_{21} A$$
$$\tilde{b} = L_{32} L_{42} L_{41} L_{31} L_{21} b$$

Step 3 Eliminate x_3 from the last equation

Fourth equation $-$ $\frac{a_{43}}{a_{33}}$. Third Equation $l_{43} = 1$

$$\tilde{A} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 2 \end{bmatrix} \qquad \tilde{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 - b_3 \end{bmatrix}$$

$$L_{43} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

$$\tilde{A} = L_{43}\, L_{32}\, L_{42}\, L_{41}\, L_{31}\, L_{21}\, A$$
$$\tilde{b} = L_{43}\, L_{32}\, L_{42}\, L_{41}\, L_{31}\, L_{21}\, b$$

The final resulting system

$$\begin{bmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 2 \end{bmatrix} * \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

(solve by backward substitution)

No need to repeat the above if A is fixed and b changes

The strategy is as follows:

$$L_{21} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ +2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$(1\ 0\ 0\ 0) \Downarrow e_1$

$\Downarrow \begin{pmatrix} 0 \\ 2 \\ 0 \\ 0 \end{pmatrix} \to 2e_2$

$$L_{21} = (I - l_{21}\, e_2\, e_1^T)$$

In general, $L_{ij} = (I - l_{ij}\, e_i\, e_j^T)$ (Note $i \neq j$)

claim L_{ij}^{-1} = same as L_{ij} except $-l_{ij}$ is replaced with l_{ij}. Precisely, $L_{ij}^{-1} = (I + l_{ij}\, e_i\, e_j^T)$

proof

$$(I - l_{ij} e_i e_j^T)(I + l_{ij} e_i e_j^T)$$
$$= I - l_{ij}^2\, e_i \underbrace{e_j^T e_i}_{=0} e_j^T \quad \text{since } i \neq j$$
$$= I$$

Next what happens when we multiply these elementary matrices?

$$L_{ij}^{-1} = (I + l_{ij}\, e_i e_j^T) \qquad L_{mn}^{-1} = (I + l_{mn}\, e_m e_n^T)$$
$$i \neq j \qquad\qquad m \neq n$$

$$L_{ij}^{-1} L_{mn}^{-1} = (I + l_{ij}\, e_i e_j^T)(I + l_{mn}\, e_m e_n^T)$$
$$= I + l_{mn}\, e_m e_n^T + l_{ij}\, e_i e_j^T + l_{ij} l_{mn} \underline{e_i e_j^T e_m e_n^T}$$
$$= \underline{\underline{I + l_{mn}\, e_m e_n^T + l_{ij}\, e_i e_j^T}} \qquad \delta_{jm}\, \underline{e_i e_n^T}$$

zero matrix unless $i = n$

claim The product of L_{ij}^{-1} and L_{mn}^{-1} is a matrix with ones on the diagonal and entries of L_{ij}^{-1} and L_{mn}^{-1} in their usual place

Exercise: Extend proof to multiple products

$$U = \tilde{A} = L_{43} L_{32} L_{42} L_{41} L_{31} L_{21} A$$
$$A = \underline{L_{21}^{-1} L_{31}^{-1} L_{41}^{-1} L_{42}^{-1} L_{32}^{-1} L_{43}^{-1}}\, U$$
$$\Downarrow$$
$$L$$

$\tilde{A}$ is upper triangular

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ 4 & 3 & 1 & 0 \\ 3 & 4 & 1 & 1 \end{bmatrix} \qquad U = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

Theorem (LU decomposition theorem)
Let $A \in \mathbb{R}^{m \times m}$ be a non-singular matrix. (No divisions by 0 occur). Then, carrying out Gaussian Elimination results L and U. Then the decomposition $A = LU$ is unique

Remark The constraint $L_{ii} = 1$ is important otherwise $A = LD^{-1}DU$ for $D \equiv$ invertible diagonal matrix works

Use of LU decomposition
$Ax = b$ (suppose we have stored L and U such that $A = LU$)
Suppose the right hand side input b changes to $\tilde{b}$
$$Ax = \tilde{b}$$
$$LUx = \tilde{b}$$
Let $y = Ux$ then $Ly = \tilde{b} \Rightarrow$ solve this for y

$$Ux = y \Rightarrow \text{ solve this for } x$$

This can be done in $O(n^2)$ computational time

Let's compare this to doing Gaussian elimination with A and $\tilde{b}$

Eliminate x_1

$m-1$ divisions

$2(m-1)$ [substraction and multiplication for each equation] $2 \le i \le m$

Total $= (m-1) + 2(m-1)^2$

Eliminate x_2

$m-2$ divisions

$2(m-2)$ [substraction and multiplication for each equation] $3 \le i \le m$

Total : $(m-2) + 2(m-2)^2$

Eliminate x_{n-1}

1 division

1 multiplication and 1 substraction

$1+2 = 3$ = Total

$$\text{Total cost} = \sum_{i=1}^{m-1} (m-i) + \sum_{i=1}^{m-1} 2(m-i)^2$$

$(m-1)+(m-2)+\dots+1$ $\qquad$ $2(m-1)^2+2(m-2)^2+\dots+2(m)^2$

(summation in reverse gives)

$$= \sum_{i=1}^{m-1} i + 2\sum_{i=1}^{m-1} i^2$$

Recall the following formulas:

$$\sum_{i=1}^{k} i = \frac{k(k+1)}{2}$$

$$\sum_{i=1}^{k} i^2 = \frac{k(k+1)(2k+1)}{6}$$

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

$$\sum_{i=1}^{m-1} i^2 = \frac{(m-1)m(2m-1)}{6}$$

$$\text{Total cost} = \frac{m(m-1)}{2} + 2\frac{(m-1)m(2m-1)}{6}$$

[After some algebra]

$$= \frac{2}{3}m^3 - \frac{1}{2}m^2 - \frac{1}{6}m$$

Important! $\qquad$ Total cost $= \frac{2}{3}n^3 + O(n^2)$

This is the main reason to precompute L and U for problems which requires solving $Ax=b$ for fixed A and varying b.

So far, no division by 0 occured. How to deal with it?

Row swapping

Assume $a_{11} = 0$

Solution: Find an i with $a_{i1} \neq 0$ and swap the first and ith equation

We continue Gaussian elimination; Now say $\tilde{a}_{22} = 0$

For $i > 2$ look for i such that $a_{i2} \neq 0$ and swap equations 2 and i

$\Rightarrow$ what happens if we find that $a_{ij} = 0$ for $i \in \{i, j+1, \dots, m\}$? We have no way of escaping 0 division.

Answer: x_j has been eliminated.

$U(j,j) = 0$

[Recall the determinant of an upper triangular matrix]

$\Rightarrow \det(U) = 0 \Rightarrow U$ is not invertible

$Ux = c$ $\Rightarrow$ no solutions, $\Rightarrow$ infinitely many solutions

$Ux = c \iff Ax = b$ [are equivalent]

$\Rightarrow A$ is singular

Main Message: Division by 0 occurs when A is singular

$a_{22} = 3.49726 \times 10^{-15}$

Find $i \in \{j, j+1, \dots m\}$ such that $|a_{ij}|$ is as large as possible

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

Partial pivoting: only swap rows

complete pivoting: also swap columns in addition to rows (not necessary in practice)

With partial pivoting, $|l_{ij}| \leq 1$

Example
$$\begin{bmatrix} 10^{-9} & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$\det(A) \approx -1$ (not singular)

$$\begin{bmatrix} 10^{-9} \\ 1 \end{bmatrix} \approx \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$l_{21} = 10^{9}$

$$\begin{bmatrix} 10^{-9} & 1 \\ 0 & 2 - 10^{+9} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 - 10^{9} \end{bmatrix}$$

The true solution is

$$x_1 \approx -1 \qquad x_2 \approx 1$$

Now with 8 digit arithmetic, Gaussian elimination gives

$$x_2 = 1 \quad \text{and} \quad x_1 = 0$$

(what we have is $\approx$ $\begin{bmatrix} 10^{-9} & 1 \\ 0 & -10^9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -10^9 \end{bmatrix}$

100% error in x_1

$\Rightarrow$ Partial pivoting $\begin{bmatrix} 1 & 2 \\ 10^{-9} & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$l_{21} = 10^{-9}$ $\begin{bmatrix} 1 & 0 \\ 0 & 1 - 2\times 10^{-9} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 - 10^{-9} \end{bmatrix}$

In 8 digit arithmetic

$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ $\quad x_2 = 1$ and $x_1 = -1$

True solution $\quad x_1 \approx 1.000000002$

$\quad x_2 \approx 1.000000001$

<u>Message</u> Without pivoting, Gaussian elimination is not backwards stable (In general)

Large $|l_{ij}|$ can cause numerical stability!

<u>Theorem</u> Let $A = LU$ be computed using Gaussian elimination without pivoting

$$\tilde{L}\tilde{U} = A + \delta A, \quad \frac{\|\delta A\|}{\|L\|\,\|U\|} = O(\varepsilon_{machine})$$

$\|L\|\,\|U\| = O(\|A\|)$ ✓

$\|L\|\,\|U\| \neq O(\|A\|)$ ✗

Without pivoting, L and U can be unboundedly large

If any hope, it is pivoting.
