System of Equations :-

Gaussian Elimination :-

$$\underset{\sim}{A}\,\underset{\sim}{x} = \underset{\sim}{b}$$

Gaussian elimination is viewed as transforming a full linear system into an upper triangular matrix, by using transformations on the left of the given system matrix $\underset{\sim}{A}$

$\rightarrow$ $\underset{\sim}{A} \in \mathbb{R}^{m \times m}$ (non-singular system matrix)

The idea is to introduce zeros below the diagonal column at a time. This is accomplished by subtracting multiples of each row from subsequent rows!

(Here L_k are lower triangular matrices)

$$\underset{\sim}{L}_{m-1}\underset{\sim}{L}_{m-2} \cdots \underset{\sim}{L}_2\,\underset{\sim}{L}_1\,\underset{\sim}{A} = \underset{\sim}{U}$$

$$\underbrace{\underset{\sim}{L}_{m-1}^{-1}\,\underset{\sim}{L}_{m-1}}_{I}\,\underset{\sim}{L}_{m-2} \cdots \underset{\sim}{L}_2\,\underset{\sim}{L}_1\,\underset{\sim}{A} = \underset{\sim}{L}_{m-1}^{-1}\,\underset{\sim}{U}$$

$$\underbrace{L_{m-2}^{-1} L_{m-1}}_{I} \cdots L_2 L_1 A = L_{m-2}^{-1} L_{m-1}^{-1} U$$

finally $\quad A = \underbrace{L_1^{-1} L_2^{-1} \cdots L_{m-1}^{-1}}\, U$

gives LU factorization of A

i.e $\boxed{A = LU}$

$L \rightarrow$ lower triangular matrix

$U \rightarrow$ upper triangular matrix

In practice, we choose L to be unit lower triangular which means all of its diagonal entries are equal to 1.

Ex:- $\quad A \in \mathbb{R}^{4\times 4}$

$$\underset{A}{\begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{bmatrix}} \xrightarrow{L_1} \underset{L_1 A}{\begin{bmatrix} \times & \times & \times & \times \\ 0 & * & * & * \\ 0 & * & * & * \\ 0 & * & * & * \end{bmatrix}}$$

$$\xrightarrow{L_2} \underset{L_1 L_2 A}{\begin{bmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & * & * \\ 0 & 0 & * & * \end{bmatrix}} \xrightarrow{L_3} \overbrace{\begin{bmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & 0 & \times & \times \\ 0 & 0 & 0 & \times \end{bmatrix}}^{L_3 L_2 L_1 A}$$

The k^{th} transformation $\underset{\sim}{L}_k$ introduces zeros below the diagonal in the column k, by subtracting multiples of row k from rows $k+1, k+2, \dots m$

Gaussian Elimination
$\longrightarrow$ triangular triangularization

Choice of L_k?

$\underset{\sim}{A} \in \mathbb{R}^{m \times m}$ (Non-singular matrix), let $\underset{\sim}{x}_k$ denote k^{th} column of the matrix at the beginning of step k.

Then L_k must be chosen such that

$$\underset{\sim}{x}_k = \left\{ \begin{bmatrix} x_{1k} \\ x_{2k} \\ \vdots \\ x_{kk} \\ x_{k+1,k} \\ \vdots \\ x_{mk} \end{bmatrix} \xrightarrow{L_k} \begin{bmatrix} x_{1k} \\ x_{2k} \\ \vdots \\ x_{kk} \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \right\}$$

To do this use subtract $l_{jk} \times$ row k from j^{th} row : $j = k+1, \dots m$

$$\boxed{l_{jk} = \frac{x_{jk}}{x_{kk}}} \quad (l_{jk} \text{ is known as multiplier})$$

Then $\underset{\sim}{L}_k = \begin{bmatrix} 1 & & & & \\ & \ddots & & & \\ & & 1 & & \\ & & -l_{k+1,k} & \ddots & \\ & & \vdots & & \\ & & -l_{m,k} & & 1 \end{bmatrix}$

Let $\underset{\sim}{l}_k = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ l_{k+1,k} \\ l_{k+2,k} \\ \vdots \\ l_{m,k} \end{bmatrix}$ Then $\underset{\sim}{L}_k = \underset{\sim}{I} - \underset{\sim}{l}_k \underset{\sim}{e}_k^T$

$\underset{\sim}{e}_k = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \to k^{th}$ entry

Verify

$$\underset{\sim}{e}_k^T \underset{\sim}{l}_k = 0$$

Consider the product $(\underset{\sim}{I} - \underset{\sim}{l}_k \underset{\sim}{e}_k^T)(\underset{\sim}{I} + \underset{\sim}{l}_k \underset{\sim}{e}_k^T)$

$$= \underset{\sim}{I} - \underset{\sim}{l}_k \underset{\sim}{e}_k^T \underset{\sim}{l}_k \underset{\sim}{e}_k^T$$

$$= \underset{\sim}{I} \quad (\text{Since } \underset{\sim}{e}_k^T \underset{\sim}{l}_k = 0)$$

Similarly consider the product

$$(\underset{\sim}{I} + \underset{\sim}{l}_k \underset{\sim}{e}_k^T)(\underset{\sim}{I} - \underset{\sim}{l}_k \underset{\sim}{e}_k^T) = \underset{\sim}{I}$$

$$\boxed{\underset{\sim}{L}_k^{-1} = \underset{\sim}{I} + \underset{\sim}{l}_k \underset{\sim}{e}_k^T}$$

$\underset{\sim}{L}_k$ matrix as defined before,

to construct $\underset{\sim}{L}_k^{-1}$, we just negate

all entries $\underset{\sim}{l}_k$

Now consider $\underset{\sim}{L}_k^{-1} \underset{\sim}{L}_{k+1}^{-1}$; $\underset{\sim}{e}_k^T \underset{\sim}{l}_{k+1} = 0$

$$\underset{\sim}{L}_k^{-1} \underset{\sim}{L}_{k+1}^{-1} = (\underset{\sim}{I} + \underset{\sim}{l}_k \underset{\sim}{e}_k^T)(\underset{\sim}{I} + \underset{\sim}{l}_{k+1} \underset{\sim}{e}_{k+1}^T)$$

$$= (\underset{\sim}{I} + \underset{\sim}{l}_k \underset{\sim}{e}_k^T + \underset{\sim}{l}_{k+1} \underset{\sim}{e}_{k+1}^T)$$

This matrix $\underset{\sim}{L}_k^{-1} \underset{\sim}{L}_{k+1}^{-1}$ is just

a matries with entries of $\underset{\sim}{L}_k^{-1}$, $\underset{\sim}{L}_{k+1}^{-1}$

merged.

$$\underset{\sim}{L} = \underset{\sim}{L}_1^{-1} \underset{\sim}{L}_2^{-1} \cdots \underset{\sim}{L}_{m-1}^{-1} = \underbrace{\begin{bmatrix} 1 & & & & 0 \\ l_{21} & 1 & & & \\ l_{31} & l_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ l_{m1} & l_{m2} & \cdots & l_{m,m-1} & 1 \end{bmatrix}}$$

Algo :- Gaussian Elimination without pivoting

$U = A$

$L = I$

for $k = 1$ to $m-1$
  for $j = k+1$ to m
    $l(j,k) = u(j,k) / u(k,k)$
    $u(j, k:m) = u(j,k:m) - l(j,k) * u(k, k:m)$ — (*)
  end for
end for

Operation count :-

The dominant experse is

$u(j,k:m) = u(j,k:m) - \underbrace{l(j,k) * u(k,k:m)}$

→ one scalar multiplication
one vector subtraction

Total flops $\approx \frac{2}{3} m^3$

* Solution of $\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$ by $\underset{\sim}{L}\underset{\sim}{U}$ factorization

$$\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$$

$$\underset{\sim}{L}\underset{\sim}{U}\underset{\sim}{x} = \underset{\sim}{b}$$

First solve $\underset{\sim}{L}\underset{\sim}{y} = \underset{\sim}{b}$ for an intermediate variable $\underset{\sim}{y}$
(forward substitution)

→ Then solve $\underset{\sim}{U}\underset{\sim}{x} = \underset{\sim}{y}$ for unknown variable $\underset{\sim}{x}$ (backward substitution)

* The initial factorization of $\underset{\sim}{A}$ into $\underset{\sim}{L}\underset{\sim}{U}$ $\sim \frac{2}{3} m^3$

* forward & backward substitution $\sim m^2$ flops

Total work to solve $\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$ by $\underset{\sim}{L}\underset{\sim}{U}$ factorization $\sim \frac{2}{3} m^3$ flops, half the amount required to solve $\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$ using Householder triangularization

Instability in Gaussian elimination:-

eg:- $\underset{\sim}{A} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$ $l_{jk} = \dfrac{x_{jk}}{x_{kk}}$

Gaussian elimination breaks down if

$x_{kk} = 0$

$K(\underset{\sim}{A}) \approx 2.618$

$\underset{\sim}{A} = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 1 \end{bmatrix}$

$\underset{\sim}{L} = \begin{pmatrix} 1 & 0 \\ 10^{20} & 1 \end{pmatrix}$ $\underset{\sim}{U} = \begin{bmatrix} 10^{-20} & 1 \\ 0 & 1-10^{20} \end{bmatrix}$

$\tilde{L} = \begin{pmatrix} 1 & 0 \\ 10^{20} & 1 \end{pmatrix}$ $\tilde{U} = \begin{bmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{bmatrix}$

$1-10^{20} = -10^{20}$

$\tilde{L}\tilde{U} = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 0 \end{bmatrix}$ This is not at all close to $\underset{\sim}{A}$

$\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$ where $\underset{\sim}{b} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ we

get $\tilde{x} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ But $x = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$
correct answer

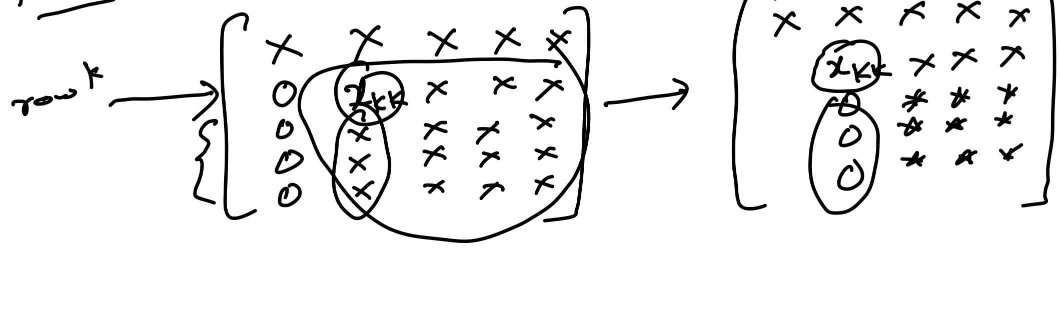
Though $\tilde{L}$ and $\tilde{U}$ are close to the true factors $\underset{\sim}{L}$ and $\underset{\sim}{U}$

But we have not been able to use $\tilde{L}$ and $\tilde{U}$ to solve $\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$ stably because using LU factorization to solve $\underset{\sim}{A}\underset{\sim}{x} = \underset{\sim}{b}$ is not stable!

Gaussian elimination with pivoting :-

* Instability of Gaussian elimination can be controlled by permuting rows of $\underset{\sim}{A}$ as we proceed.

Pivots :



This x_{kk} is called piv

we could zero out other entries $(k < i \leq m)$

$k=2 \quad i=4$

$$\begin{bmatrix} x & x & x & x & x \\ & x & x & x & x \\ & x & x & x & x \\ & x_{ik} & x & x & x \\ & x & x & x & x \end{bmatrix} \longrightarrow \begin{bmatrix} x & x & x & x & x \\ & 0 & * & * & * \\ & 0 & * & * & * \\ & x_{ik} & x & x & x \\ & 0 & * & * & * \end{bmatrix}$$

We could also zero out entries in colum j instead of k $(k < j \leq m)$

eg: $\underline{k=2}$ $i=4, j=3$

$$\begin{bmatrix} x & x & x & x & x \\ & x & x & x & x \\ & x & x & x & x \\ & x & x_{ij} & x & x \\ & x & x & x & x \end{bmatrix} \longrightarrow \begin{bmatrix} x & x & x & x & x \\ & * & 0 & * & * \\ & * & 0 & * & * \\ & x & x_{ij} & x & x \\ & * & 0 & * & * \end{bmatrix}$$

We can choose any entry $x(k:m, k:m)$ as pivot as long is not zero!

→ After choosing x_{ij} as pivot, interchange rows and columns of the matrix so that x_{ij} takes the position of x_{kk}.

→ Every entry in $X(k:m, k:m)$ as a possible pivot at step k, then we must examine $(m-k+1)^2$ elements and choose largest so that total number of elements examined

$$= \sum_{k=1}^{m-1} (m-k+1)^2 \simeq O(m^3)$$

If you choose the pivot in the above way, it is called complete pivoting!

Hence we do partial pivoting and we only search for elements in column k for the largest one! For a given k, $(m-k+1)$ elements need to be searched!

Total number of elements examined

$$\sum_{k=1}^{m-1} (m-k+1) = O(m^2)$$

eg:- $\underset{\sim}{P} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$ $\underset{\sim}{P}\underset{\sim}{A}$ $= (\underset{\sim}{A}$ with 2nd and 3rd rows permuted)

The k^{th} step of Gaussian elimination with partial pivoting can be viewed as:

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & x_{kk} & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix} \xrightarrow{P_k} \begin{bmatrix} \times & \times & \times & \times & \times \\ & x_{ik} & * & * & * \\ & \times & \times & \times & \times \\ & * & * & * & * \\ & \times & \times & \times & \times \end{bmatrix}$$

pivot selection

row interchange

$$\xrightarrow{L_k} \begin{bmatrix} \times & \times & \times & \times & \times \\ & x_{ik} & \times & \times & \times \\ & 0 & * & * & * \\ & 0 & * & * & * \\ & 0 & * & * & * \end{bmatrix}$$

$$L_{m-1}P_{m-1}\cdots L_2P_2L_1P_1A = U$$

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

Interchange 1^{st} and 3^{rd} row

(Left multiply A with P_1)

$$\underset{P_1}{\begin{bmatrix}0&0&1&0\\0&1&0&0\\1&0&0&0\\0&0&0&1\end{bmatrix}}\underset{A}{\begin{bmatrix}2&1&1&0\\4&3&3&1\\8&7&9&5\\6&7&9&8\end{bmatrix}} = \underset{P_1A}{\begin{bmatrix}8&7&9&5\\4&3&3&1\\2&1&1&0\\6&7&9&8\end{bmatrix}}$$

$$\underset{L_1}{\begin{bmatrix}1&&&0\\-1/2&1&&\\-1/4&&1&\\-3/4&&0&1\end{bmatrix}}\underset{P_1A}{\begin{bmatrix}8&7&9&5\\4&3&3&1\\2&1&1&0\\6&7&9&8\end{bmatrix}} = \underset{L_1P_1A}{\begin{bmatrix}8&7&9&5\\0&-1/2&-3/2&-3/2\\0&-3/4&-5/4&-5/4\\0&7/4&9/4&17/4\end{bmatrix}}$$

Left multiply L_1P_1A with P_2

$$\underbrace{L_3P_3L_2P_2L_1P_1}A = U$$

$$\underset{\sim}{U} = \begin{bmatrix}8&7&9&5\\&7/4&9/4&17/4\\&0&-6/7&-2/7\\&&&2/3\end{bmatrix}$$

$$\underset{\sim}{L}\cdot\underset{\sim}{U} = \underset{\sim}{P}\underset{\sim}{A}$$

$$\underbrace{L_3P_3L_2P_2L_1P_1}A = U$$

$$= \underset{\sim}{L_3'}\,\underset{\sim}{L_2'}\,\underset{\sim}{L_1'}\,P_3P_2P_1$$

$$L_3' = L_3;\quad L_2' = P_3L_2P_3^{-1};$$

$$L_1' = \underbrace{P_3P_2L_1P_2^{-1}P_3^{-1}}$$

$$\underbrace{L_3 P_3 L_2 P_2 L_1 P_1} = L_3 \underline{(P_3 L_2 P_3^{-1})} \underline{(P_3 P_2 L_1 P_2^{-1} P_3^{-1})} P_3 P_2 P_1$$

In general $m \times m$ case Gaussian elimination with partial pivoting can be written as

$$\underbrace{(L'_{m-1} L'_{m-2} \cdots L'_2 L'_1)} (P_{m-1} P_{m-2} \cdots P_2 P_1) A = U$$

where $L'_k = P_{m-1} \cdots P_{k+1} L_k P_{k+1}^{-1} \cdots P_{m-1}^{-1}$

and write

$$L = (L'_{m-1} L'_{m-2} \cdots L'_2 L'_1)^{-1} \text{ and } P$$

as $P = \underbrace{P_{m-1} P_{m-2} \cdots P_2 P_1}$

we have $PA = LU$

L is unit lower triangular and elements of L satisfy $|L_{ij}| \le 1$ and U is upper triangular

"Permute matrix $\underset{\sim}{A}$ ahead of time using matrix $\underset{\sim}{P}$ and then apply Gaussian elimination to this permuted matrix."

<u>Thm</u>:- Let $\underset{\sim}{A} \in \mathbb{R}^{m\times m}$ non-singular matrix, compute $\underset{\sim}{A} = \underset{\sim}{L}\underset{\sim}{U}$ by Gaussian elimination process, then the computed matrices $\tilde{L}, \tilde{U}$ satisfy

$$\underset{\sim}{\tilde{L}}\,\underset{\sim}{\tilde{U}} = \underset{\sim}{A} + \underset{\sim}{\delta A}, \quad \frac{\|\delta A\|}{\|L\|\,\|U\|} = O(\varepsilon_M)$$

(if $\underset{\sim}{A}$ has successful LU factorization without encountering zero pivots)

<u>Remarks</u>:-

(1) If $\|L\|$ and/or $\|U\|$ is large relative to $\|A\|$, then you

$$\frac{\|\delta A\|}{\|A\|} \neq O(\varepsilon_M)$$

(2) If $\|L\|\|U\| = O(\|A\|)$ then Gaussian elimination is backward stable!

(3) Idea behind pivoting is to make sure $\|L\|, \|U\|$ are not too large

For partial pivoting,

→ the elements of $\underset{\sim}{L}$ all satisfy $|l_{ij}| \leq 1$

→ $\|L\| = O(1)$

→ The condition $\dfrac{\|\delta A\|}{\|L\|\|U\|} = O(\varepsilon_M)$ for backward stability of Gaussian elimination with partial pivoting reduce to $\dfrac{\|\delta A\|}{\|U\|} = O(\varepsilon_M)$, this algo is backward stable provided $\underbrace{\|\underset{\sim}{U}\| = O(\|\underset{\sim}{A}\|)}$

To study stability of Gaussian elimination with partial pivoting we define growth factor for $\underset{\sim}{A}$ as

$$\rho = \frac{\max_{ij} |u_{ij}|}{\max_{ij} |a_{ij}|}$$

If $\rho = O(1)$, elimination process is stable.

This definition of ρ implies

$$\|U\| = O(\rho \|A\|) \text{ and}$$

Thm: Suppose we compute $\underline{P}\underline{A} = \underline{L}\underline{U}$ for a given $\underset{\sim}{A} \in \mathbb{R}^{m \times m}$, then computed matrices $\tilde{P}, \tilde{L}, \tilde{U}$ satisfy

$$\underline{\tilde{L}}\,\underline{\tilde{U}} = \underline{\tilde{P}}\underline{A} + \underline{\delta A} \quad \text{where}$$

$$\frac{\|\delta A\|}{\|A\|} = O(\rho\, \varepsilon_M) \text{ for some } \underset{\sim}{\delta A} \in \mathbb{R}^{m \times n}$$

* Gaussian elimination with partial pivoting is backward stable if $\rho = O(1)$

uniformly for all matrices of a dimension m, otherwise it is not