Pivoting

It may happen that some pivot elements are zero even though matrix A is nonsingular. If this is the case, then the above procedure breaks down.

Ex

$$\left(\underbrace{\begin{array}{ccc} 1 & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 2 & 2 \end{array}}_{A}\left|\begin{array}{c} 1 \\ 2 \\ 1 \end{array}\right.\right)$$

$\det A = -1 \neq 0 \Rightarrow A$ is nonsingular

$$\left(\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 2 \\ 1 & 2 & 2 & 1 \end{array}\right) \qquad m_{21} = \frac{1}{1} = 1, \quad m_{31} = \frac{1}{1} = 1$$

University of Idaho

$$\left(\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & \boxed{0} & 1 & 1 \\ 0 & 1 & 1 & 0 \end{array}\right)$$

$a_{22}^{(2)} = 0$ even though $\det A = -1 \neq 0$

$m_{31} = \frac{1}{0}$

<u>Remedy</u>: interchange rows 2 and 3 and proceed.

$$\left(\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{array}\right)$$

$x_3 = 1/1 = 1$

$x_2 = (0 - 1 \cdot \underbrace{x_3}_{1})/1 = -1$

$x_1 = 1$

$$\Rightarrow \quad x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$$

General case

Suppose matrix A is invertible but some pivot $a_{kk}^{(k)} = 0$

$$A^{(k)} = E_{k-1} \dots E_2 E_1 A = \begin{pmatrix} a_{11}^{(1)} & \dots & a_{1k}^{(1)} & \dots & a_{1n}^{(1)} \\ & \ddots & & & \\ & & a_{kk}^{(k)} = 0 & \dots & a_{kn}^{(k)} \\ & 0 & \vdots & & \vdots \\ & & a_{nk}^{(k)} & \dots & a_{nn}^{(k)} \end{pmatrix}$$

$$\det A^{(k)} = \underbrace{\det E_{k-1}}_{=1} \underbrace{\det E_{k-2}}_{=1} \dots \underbrace{\det E_2}_{=1} \underbrace{\det E_1}_{=1} \cdot \underbrace{\det A}_{\neq 0} = \det A \neq 0$$

$\Rightarrow \det A^{(k)} \neq 0 \Rightarrow A^{(k)}$ is also invertible. If $a_{ik}^{(k)} = 0$, $i = k+1, \dots, n$, then one can show that the first k columns of $A^{(k)}$ are linearly dependent, which contradicts the fact that $A^{(k)}$ is invertible. Let i be the first row in which $a_{ik}^{(k)} \neq 0$. Then switch rows k and i and proceed.

$$A^{(k)} \longrightarrow P_k A^{(k)}, \qquad P_k : \text{permutation matrix}$$

$$\begin{array}{cc}
P_k = \begin{pmatrix}
1 & & & & & & & \\
& \ddots & & & & & & \\
& & 1 & & & & & \\
& & & 0 & \cdots & 1 & & \\
& & & \vdots & 1 \;\ddots\; 1 & \vdots & & \\
& & & 1 & \cdots & 0 & & \\
& & & & & & 1 & \\
& & & & & & & \ddots \;\; 1
\end{pmatrix} & \begin{array}{l} \\ \\ \\ \text{row } k \\ \\ \text{row } i \\ \\ \\ \end{array} \\
\qquad\qquad \text{col. } k \quad \text{col. } i &
\end{array}$$

<u>Note</u> $\det P_k = -1$

<u>Thm</u> Let A be nonsingular. Then there exists a permutation matrix P such that $PA = LU$ where L is unit lower triangular matrix, U is upper triangular matrix.

Pf

We can pivot to produce

$$E_{n-1}P_{n-1}\ \ldots\ E_2P_2E_1P_1A = U = \begin{pmatrix} a_{11}^{(1)} & \cdots & a_{1n}^{(1)} \\ & \ddots & \\ 0 & & a_{nn}^{(n)} \end{pmatrix}$$

Some P_i may be identity matrices.

In general, $P_2E_1 \neq E_1P_2$. But there exists another transformation matrix $\tilde{E}_1$ such that

$$P_2E_1 = \tilde{E}_1P_2$$

Then

$$\tilde{E}_{n-1}\ \ldots\ \tilde{E}_2\tilde{E}_1 \underbrace{P_{n-1}\ \ldots\ P_2P_1}_{P} A = U$$

$$\underbrace{P_{n-1} \dots P_2 P_1}_{P} A = \left(\tilde{E}_{n-1} \dots \tilde{E}_2 \tilde{E}_1\right)^{-1} U$$

$$\underbrace{P_{n-1} \dots P_2 P_1}_{P} A = \underbrace{\tilde{E}_1^{-1} \tilde{E}_2^{-1} \dots \tilde{E}_{n-1}^{-1}}_{L} U$$

$$\Rightarrow \boxed{PA = LU}$$

Note

1. P contains pivoting information: in practice it is not necessary to store matrix P, the information can be stored in the integer pivotal array (~~vector~~)

$$P = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$p(1) = 3$
$p(2) = 1$
$p(3) = 2$

$$\Rightarrow \quad p = \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix}$$

2. Since $\det P_k = \pm 1 \Rightarrow \det A = \pm a_{11}^{(1)} a_{22}^{(2)} \cdots a_{nn}^{(n)}$

Def Matrix A is called <u>strictly diagonally dominant</u>

if $|a_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}| \qquad i = 1, \dots, n$

Def Matrix A is called <u>positive definite</u> if $x^T A x > 0$

for all $x \neq 0$.

3. $A_k = \begin{pmatrix} a_{11} & \cdots & a_{1k} \\ \vdots & & \vdots \\ a_{k1} & \cdots & a_{kk} \end{pmatrix}$: $k \times k$ leading submatrix of A

Thm If matrix A is strictly diagonally dominant or A is positive definite or determinants of all leading submatrices $\det A_k \neq 0$, then pivots arising in

Gaussian elimination are nonzero and pivoting is not needed, i.e. $A = LU$

Note In practice, pivoting is recommended when pivot is small.

Ex
$$\left(\begin{array}{cc|c} \varepsilon & 1 & 1+\varepsilon \\ 1 & 1 & 2 \end{array}\right) \qquad m_{21} = \frac{1}{\varepsilon}$$

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

$$\left(\begin{array}{cc|c} \varepsilon & 1 & 1+\varepsilon \\ 0 & 1-\frac{1}{\varepsilon} & 1-\frac{1}{\varepsilon} \end{array}\right) \uparrow$$

$$\left.\begin{array}{l} x_2 = \left(1-\frac{1}{\varepsilon}\right) / \left(1-\frac{1}{\varepsilon}\right) = 1 \\ x_1 = \left(1+\varepsilon - 1\cdot \underset{=1}{x_2}\right)/\varepsilon = (1+\varepsilon-1)/\varepsilon = 1 \end{array}\right\} \text{exact solution}$$

University of Idaho

Now, due to rounding, the reduced system will look like

$$\left(\begin{array}{cc|c} \varepsilon & 1 & 1 \\ 0 & -\frac{1}{\varepsilon} & -\frac{1}{\varepsilon} \end{array}\right)$$

$\tilde{x}_2 = 1$

$\tilde{x}_1 = (1 - 1\cdot\tilde{x}_2)/\varepsilon = (1 - 1.1)/\varepsilon = 0$

$\Rightarrow \tilde{x} = \begin{pmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

computed solution is inaccurate

<u>Remedy</u>: pivot, even if $a_{11} \neq 0$

$$\left(\begin{array}{cc|c} 1 & 1 & 2 \\ \varepsilon & 1 & 1+\varepsilon \end{array}\right)$$

Due to rounding we have

$$\left(\begin{array}{cc|c} 1 & 1 & 2 \\ \varepsilon & 1 & 1 \end{array}\right) \qquad m_{21} = \frac{\varepsilon}{1} = \varepsilon$$

$$\left(\begin{array}{cc|c} 1 & 1 & 2 \\ 0 & 1-\varepsilon & 1-2\varepsilon \end{array}\right) \overset{\text{round}}{\approx} \left(\begin{array}{cc|c} 1 & 1 & 2 \\ 0 & 1 & 1 \end{array}\right) \uparrow$$

$$\tilde{x}_2 = 1$$

$$\tilde{x}_1 = (2 - 1 \cdot \tilde{x}_2)/1 = (2-1)/1 = 1 \qquad \Rightarrow \tilde{x} = \begin{pmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

new computed solution is accurate!

Partial pivoting

Choose i such that

$$|a_{ik}^{(k)}| = \max\{|a_{kk}^{(k)}|, |a_{k+1,k}^{(k)}|, \dots, |a_{nk}^{(k)}|\}$$

University of Idaho

Then interchange rows i and k.

Scaled Partial Pivoting

Choose i such that

$$\frac{|a_{ik}^{(k)}|}{s_i} = \max\left\{ \frac{|a_{kk}^{(k)}|}{s_k}, \frac{|a_{k+1,k}^{(k)}|}{s_{k+1}}, \dots, \frac{|a_{nk}^{(k)}|}{s_n} \right\}$$

where

$$s_r = \max\{ |a_{r,k}^{(k)}|, |a_{r,k+1}^{(k)}|, \dots, |a_{rn}^{(k)}| \}$$

Using partial or scaled partial pivoting lets one keep the error in reduced matrices $A^{(k)}$ at the same order as error in the original matrix. A.