Numerical Analysis

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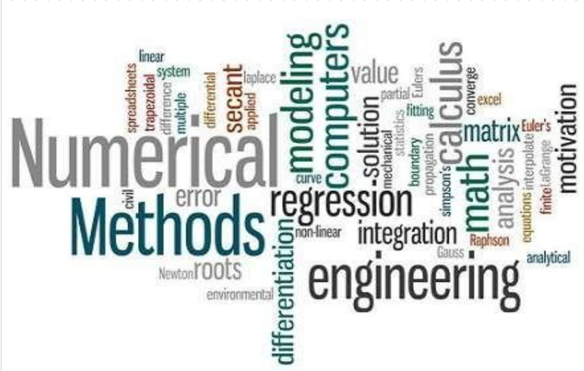

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Course Syllabus

- **Introduction:** Numerical analysis and background, definitions of computer number systems, floating point representation, representation of numbers in different bases, and round-off errors.
- **Root Finding:** Bisection method, fixed-point iteration, Newton's method, the secant method and their error analysis and order of convergence (Newton’s method and Secant method).
- **Direct Methods for Solving Linear Systems:** Gaussian elimination, LU decomposition, pivoting strategies, and PA=LU-factorization,…..
- **Polynomial:** Polynomial interpolation, piecewise linear interpolation, cubic spline interpolation, and curve fitting in interpolation (Application: Regression)…...
- **Integration:** Numerical differentiation, numerical integration, and composite numerical integration…….
- **Ordinary Differential Equations:** Euler's Method, and Runge-Kutta methods…..

- **Partial Pivoting method**

- **Permutation Matrices**

- **PA= LU Factorization**

Partial Pivoting Method

- The first step is to use the diagonal element a_{11} as a pivot to eliminate the first column.
- The **partial pivoting** protocol consists of comparing numbers before carrying out each elimination step.
- The largest entry of the first column is located, and its row is swapped with the pivot row, in this case the top row.
- In other words, at the start of Gaussian elimination, partial pivoting asks that we select the pth row, where

$$|a_{p1}| \geq |a_{i1}|$$

for all $1 \leq i \leq n$, and exchange rows 1 and p. Next, elimination of column 1 proceeds as usual, using the “new” version of a_{11} as the pivot.

Partial Pivoting Method

- When deciding on the second pivot, we start with the current a_{22} and check all entries directly below. We select the row p such that

$$|a_{p2}| \geq |a_{i2}|$$

for all $2 \leq i \leq n$, and if $p \neq 2$, rows 2 and p are exchanged. Row 1 is never involved in this step. If $|a_{22}|$ is already the largest, no row exchange is made.

Benefits of Partial Pivoting:

- Prevents division by 0 when $u_{ii} = 0$
- Reduce round-off errors

Partial Pivoting Method

Working Rule

Consider the system of equation

$$a_1x + b_1y + c_1z = d_1$$
$$a_2x + b_2y + c_2z = d_2$$
$$a_3x + b_3y + c_3z = d_3$$

1. Write the matrix form of systems of equations

$$\begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}$$

2. Find Augmented matrix for given system.

$$C = [A\colon B]$$

3. Transform augmented matrix 'C' into upper triangular form/ echelon form

$$\left[\begin{array}{ccc:c} a_1 & b_1 & C_1 & d_1 \\ 0 & b_2 & C_2 & d_2 \\ 0 & 0 & C_3 & d_3 \end{array}\right]$$

→Find 1st Pivot element. (left column).

→ Complete first pass.

→ Find 2nd Pivot element.

→ Complete 2nd Pass.

4. Write system of equations

5. Using back substitution, find solution of given system of equations

Partial Pivoting Method

Apply Gaussian elimination with partial pivoting to solve the system

$$\begin{aligned} x_1 - x_2 + 3x_3 &= -3 \\ -x_1 - 2x_3 &= 1 \\ 2x_1 + 2x_2 + 4x_3 &= 0. \end{aligned}$$

This example is written in tableau form as

$$\left[\begin{array}{rrr|r} 1 & -1 & 3 & -3 \\ -1 & 0 & -2 & 1 \\ 2 & 2 & 4 & 0 \end{array}\right]$$

Under partial pivoting

$$\left[\begin{array}{rrr|r} 1 & -1 & 3 & -3 \\ -1 & 0 & -2 & 1 \\ 2 & 2 & 4 & 0 \end{array}\right] \longrightarrow \begin{array}{c}\text{exchange row 1}\\ \text{and row 3}\end{array} \longrightarrow \left[\begin{array}{rrr|r} 2 & 2 & 4 & 0 \\ -1 & 0 & -2 & 1 \\ 1 & -1 & 3 & -3 \end{array}\right]$$

Partial Pivoting Method

$$\left[\begin{array}{rrr|r} 2 & 2 & 4 & 0 \\ -1 & 0 & -2 & 1 \\ 1 & -1 & 3 & -3 \end{array}\right] \rightarrow \begin{array}{c}\text{subtract } -\frac{1}{2}\times \text{row 1} \\ \text{from row 2}\end{array} \longrightarrow \left[\begin{array}{rrr|r} 2 & 2 & 4 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & -1 & 3 & -3 \end{array}\right] \rightarrow \begin{array}{c}\text{subtract } \frac{1}{2}\times \text{row 1} \\ \text{from row 3}\end{array}$$

$$\rightarrow \left[\begin{array}{rrr|r} 2 & 2 & 4 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & -2 & 1 & -3 \end{array}\right]. \longrightarrow \begin{array}{c}\text{exchange row 2} \\ \text{and row 3}\end{array} \longrightarrow \left[\begin{array}{rrr|r} 2 & 2 & 4 & 0 \\ 0 & -2 & 1 & -3 \\ 0 & 1 & 0 & 1 \end{array}\right]$$

$$\longrightarrow \begin{array}{c}\text{subtract } -\frac{1}{2}\times \text{row 2} \\ \text{from row 3}\end{array} \longrightarrow \left[\begin{array}{rrr|r} 2 & 2 & 4 & 0 \\ 0 & -2 & 1 & -3 \\ 0 & 0 & \frac{1}{2} & -\frac{1}{2} \end{array}\right].$$

The equations are now simple to solve. From

$$\frac{1}{2}x_3 = -\frac{1}{2}$$

$$-2x_2 + x_3 = -3$$

$$2x_1 + 2x_2 + 4x_3 = 0,$$

We found that

$$x_1 = 1$$
$$x_2 = 1$$
$$x_3 = -1$$

Partial Pivoting Method

Example:

$$\begin{bmatrix} 0 & 1 & 2 & 3 \\ 0 & 1 & 4 & 12 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -0.2 \\ 0.8 \\ 1.5 \\ 1.2 \end{bmatrix}$$

$$\begin{array}{cc} & \xrightarrow{\quad j \quad} \\ i \downarrow & \begin{bmatrix} 0 & 1 & 2 & 3 & -0.2 \\ 0 & 1 & 4 & 12 & 0.8 \\ 1 & 1 & 1 & 1 & 1.5 \\ 1 & 2 & 4 & 8 & 1.2 \end{bmatrix} \end{array}$$

Create the augmented matrix $[\mathbf{A}\ ,\ \mathbf{B}]$

$$\begin{bmatrix} 0 & 1 & 2 & 3 & -0.2 \\ 0 & 1 & 4 & 12 & 0.8 \\ 1 & 1 & 1 & 1 & 1.5 \\ 1 & 2 & 4 & 8 & 1.2 \end{bmatrix}$$

diagonal location $k = 1$

$$\begin{array}{cc} & \xrightarrow{\quad j \quad} \\ i \downarrow & \begin{bmatrix} 0 & 1 & 2 & 3 & -0.2 \\ 0 & 1 & 4 & 12 & 0.8 \\ 1 & 1 & 1 & 1 & 1.5 \\ 1 & 2 & 4 & 8 & 1.2 \end{bmatrix} \end{array}$$

Partial pivot:

- Search all rows > k for the highest magnitude
- If needed, swap row k with the highest magnitude row

Partial Pivoting Method

After first pivoting

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1.5 \\ 0 & 1 & 4 & 12 & 0.8 \\ 0 & 1 & 2 & 3 & -0.2 \\ 1 & 2 & 4 & 8 & 8 \end{bmatrix}$$

diagonal location $k = 1$

$$\begin{array}{cc} & \xrightarrow{\;j\;} \\ \downarrow i & \begin{bmatrix} 1 & 1 & 1 & 1 & 1.5 \\ 0 & 1 & 4 & 12 & 0.8 \\ 0 & 1 & 2 & 3 & -0.2 \\ 1 & 2 & 4 & 8 & 1.2 \end{bmatrix} \end{array} \quad \begin{array}{l} R_2 - 0R_1 \\ R_3 - 0R_1 \\ R_4 - 1R_1 \end{array} \longrightarrow \begin{bmatrix} 1 & 1 & 1 & 1 & 1.5 \\ 0 & 1 & 4 & 12 & 0.8 \\ 0 & 1 & 2 & 3 & -0.2 \\ 0 & 1 & 3 & 7 & -0.3 \end{bmatrix}$$

Elimination pass on all rows $i > k$:

$$a_{21} / a_{11} = 0/1 = 0$$

$$a_{31} / a_{11} = 0/1 = 0$$

$$a_{41} / a_{11} = 1/1 = 1$$

diagonal location $k = 2$

$$\begin{array}{cc} & \xrightarrow{\;j\;} \\ \downarrow i & \begin{bmatrix} 1 & 1 & 1 & 1 & 1.5 \\ 0 & 1 & 4 & 12 & 0.8 \\ 0 & 1 & 2 & 3 & -0.2 \\ 0 & 1 & 3 & 7 & -0.3 \end{bmatrix} \end{array} \quad \begin{array}{l} R_3 - 1R_2 \\ \\ R_4 - 1R_2 \end{array}$$

Partial pivot:
- Search all rows > 2 for the highest magnitude
- If needed, swap row 2 with the highest magnitude row

Elimination pass on all rows $i > 2$:

$$a_{32} / a_{22} = 1/1 = 1$$

$$a_{42} / a_{22} = 1/1 = 1$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1.5 \\ 0 & 1 & 4 & 12 & 0.8 \\ 0 & 0 & -2 & -9 & -1.0 \\ 0 & 0 & -1 & -5 & -1.1 \end{bmatrix}$$

Partial Pivoting Method

diagonal location $k = 3$

$$\begin{array}{cc} & j \\ i & \begin{bmatrix} 1 & 1 & 1 & 1 & 1.5 \\ 0 & 1 & 4 & 12 & 0.8 \\ 0 & 0 & -2 & -9 & -1.0 \\ 0 & 0 & -1 & -5 & -1.1 \end{bmatrix} \end{array}$$

$$\Big\downarrow\; R_4 - (0.5)R_3$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1.5 \\ 0 & 1 & 4 & 12 & 0.8 \\ 0 & 0 & -2 & -9 & -1.0 \\ 0 & 0 & 0 & -0.5 & -0.6 \end{bmatrix}$$

Partial pivot:

- Search all rows > 3 for the highest magnitude
- If needed, swap row 3 with the highest magnitude row

Elimination pass on all rows $i > 3$:

$$a_{43} / a_{33} = -1/-2 = 0.5$$

Implement backward substitution

$$\begin{array}{cc} & j \\ i & \begin{bmatrix} 1 & 1 & 1 & 1 & 1.5 \\ 0 & 1 & 4 & 12 & 0.8 \\ 0 & 0 & -2 & -9 & -1.0 \\ 0 & 0 & 0 & -0.5 & -0.6 \end{bmatrix} \end{array}$$

$$\mathbf{U} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 4 & 12 \\ 0 & 0 & -2 & -9 \\ 0 & 0 & 0 & -0.5 \end{bmatrix} \qquad \mathbf{C} = \begin{bmatrix} 1.5 \\ 0.8 \\ -1.0 \\ -0.6 \end{bmatrix}$$

$$\begin{aligned} x_1 + x_2 + x_3 + x_4 &= 1.5 \\ x_2 + 4x_3 + 12x_4 &= 0.8 \\ -2x_3 - 9x_4 &= -1.0 \\ -0.5x_4 &= -0.6 \end{aligned}$$

$$x_1 = -0.8 \qquad x_3 = -4.9$$
$$x_2 = 6.0 \qquad x_4 = 1.2$$

Partial Pivoting Method

Check if round-off error is significant

$$\begin{bmatrix} 0 & 1 & 2 & 3 \\ 0 & 1 & 4 & 12 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -0.2 \\ 0.8 \\ 1.5 \\ 1.2 \end{bmatrix}$$

$$x_1 = -0.8$$
$$x_2 = 6.0$$
$$x_3 = -4.9$$
$$x_4 = 1.2$$

$$\max_{1 \le i \le n} \left| \sum_{j=1}^{n} a_{ij} x_j - b_i \right| \overset{?}{<} \varepsilon$$

Error for equation $i = 1$,

$$\left| 0x_1 + 1x_2 + 2x_3 + 3x_4 - (-0.2) \right| = \left| 0(-0.8) + 1(6.0) + 2(-4.9) + 3(1.2) + 0.2 \right| = 0$$

Using MATLAB $\to 0.17\mathrm{E}-15$

Permutation Matrices

- Permutation Matrix: A matrix, P, such that P is a square matrix made up of only ones and zeros and each row and column have exactly one 1.

$$P=\begin{bmatrix}0 & 0 & 1\\ 1 & 0 & 0\\ 0 & 1 & 0\end{bmatrix} \qquad P=\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{bmatrix}$$

- Permutation matrices are similar to the identity matrix in that when you multiply by it, the values don't change

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

- Permutation matrices are different to the identity matrix in that they rearrange the rows or the columns of the matrix.

Permutation Matrices

How to use Permutation Matrices

For some matrix A and permutation matrix P,

- $P \times A$ is a row permutation
  - This will rearrange the rows of A
  - Rows always go before columns, so if P is before, it's a row permutation
- $A \times P$ is a column permutation
  - This will rearrange the columns of A
- If P is a row permutation matrix,
  - Then, if $P_{i.j} = 1$, row j is moved to row i
- If P is a column permutation matrix,
  - Then, if $P_{i,j} = 1$, column i is moved to column j

Permutation Matrices

How to use Permutation Matrices

Ex 1:= A $= \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}, P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$, calculate P$\times$ A and describe the transformations.

$$\text{P x A} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \text{ x } \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$$

$$\text{P x A} = \begin{bmatrix} 3 & 4 \\ 5 & 6 \\ 1 & 2 \end{bmatrix}$$

Transformations:

$p_{1,2} = 1$, so row 2 goes to row 1

$p_{2,3} = 1$, so row 3 goes to row 2

$p_{3,1} = 1$, so row 1 goes to row 3

Permutation Matrices

How to use Permutation Matrices

$Ex\ 1$: $A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$ create a matrix product which results in the matrix $\begin{bmatrix} 3 & 1 & 2 \\ 6 & 4 & 5 \end{bmatrix}$

Columns have been rearranged, so we are looking for $A \times P$

Since A is 2×3 , so since P is square P is a (3×3)

$$A \text{ x } P = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \times \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

$$So\ P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

Transformations:

Column 1 goes to column 2, so $p_{12} = 1$

Column 2 goes to column 3, so $p_{23} = 1$

Column 3 goes to column 1, so $p_{31} = 1$

$$A \text{ x } P = \begin{bmatrix} 3 & 1 & 2 \\ 6 & 4 & 5 \end{bmatrix}$$

PA= LU Factorization

- This is the matrix formulation of elimination with partial pivoting. The PA= LU factorization is the established workhorse for solving systems of linear equations.

- The PA= LU factorization is simply the LU factorization of a row-exchanged version of A.

- Under partial pivoting, the rows that need exchanging are not known at the outset, so we must be careful about fitting the row exchange information into the factorization.

- In particular, we need to keep track of previous multipliers when a row exchange is made. We begin with an example.

Example: Find the PA= LU factorization of the matrix

$$A = \begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix}.$$

PA= LU Factorization

First, rows 1 and 2 need to be exchanged, according to partial pivoting:

$$\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix} \xrightarrow{P = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}} \text{exchange rows 1 and 2} \longrightarrow \begin{bmatrix} 4 & 4 & -4 \\ 2 & 1 & 5 \\ 1 & 3 & 1 \end{bmatrix}.$$

We will use the permutation matrix P to keep track of the cumulative permutation of rows that have been done along the way. Now we perform two row operations, namely,

$$\longrightarrow \begin{array}{c} \text{subtract } \frac{1}{2} \times \text{ row 1} \\ \text{from row 2} \end{array} \longrightarrow \begin{bmatrix} 4 & 4 & -4 \\ \frac{1}{2} & -1 & 7 \\ 1 & 3 & 1 \end{bmatrix} \longrightarrow \begin{array}{c} \text{subtract } \frac{1}{4} \times \text{ row 1} \\ \text{from row 3} \end{array} \longrightarrow \begin{bmatrix} 4 & 4 & -4 \\ \frac{1}{2} & -1 & 7 \\ \frac{1}{4} & 2 & 2 \end{bmatrix},$$

To eliminate the first column, we have done something new—instead of putting only a zero in the eliminated position, we have made the zero a storage location. Inside the zero at the (i, j) position, we store the multiplier m_{ij} that we used to eliminate that position. We do this for a reason. This is the mechanism by which the multipliers will stay with their row, in case future row exchanges are made.

PA= LU Factorization

- Next we must make a comparison to choose the second pivot. Since $|a_{22}| = 1 < 2 = |a_{32}|$, a row exchange is required before eliminating the second column. Notice that the previous multipliers move along with the row exchange:

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

$$\xrightarrow{\text{exchange rows 2 and 3}} \begin{bmatrix} 4 & 4 & -4 \\ \frac{1}{4} & 2 & 2 \\ \frac{1}{2} & -1 & 7 \end{bmatrix}$$

- Finally, the elimination ends with one more row operation:

$$\xrightarrow{\substack{\text{subtract } -\frac{1}{2} \times \text{row 2} \\ \text{from row 3}}} \begin{bmatrix} 4 & 4 & -4 \\ \frac{1}{4} & 2 & 2 \\ \frac{1}{2} & -\frac{1}{2} & 8 \end{bmatrix}.$$

This is the finished elimination. Now we can read off the PA= LU factorization:

$$\underbrace{\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}}_{P}\underbrace{\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{4} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 1 \end{bmatrix}}_{L}\underbrace{\begin{bmatrix} 4 & 4 & -4 \\ 0 & 2 & 2 \\ 0 & 0 & 8 \end{bmatrix}}_{U} \longrightarrow \text{Eq 1}$$

PA= LU Factorization

Using the PA= LU factorization to solve a system of equations Ax = b is just a slight variant of the A = LU version. Multiply through the equation Ax = b by P on the left, and then proceed as before:

$$PAx = Pb$$
$$LUx = Pb. \longrightarrow \text{Eq 2}$$

Solve

1. $Lc = Pb$ for c. $\longrightarrow$ Eq 3
2. $Ux = c$ for x.

Example: Use the PA= LU factorization to solve the system Ax = b, where

$$A = \begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix}, \quad b = \begin{bmatrix} 5 \\ 0 \\ 6 \end{bmatrix}.$$

The PA= LU factorization is known from eq 1. It remains to complete the two back substitutions.

1. $Lc = Pb$:

$$\begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{4} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 5 \\ 0 \\ 6 \end{bmatrix} = \begin{bmatrix} 0 \\ 6 \\ 5 \end{bmatrix}.$$

PA= LU Factorization

Starting at the top, we have

$c_1 = 0$ $\quad \frac{1}{4}(0) + c_2 = 6 \Rightarrow c_2 = 6$ $\quad \frac{1}{2}(0) - \frac{1}{2}(6) + c_3 = 5 \Rightarrow c_3 = 8.$

2. $Ux = c$:

$$\begin{bmatrix} 4 & 4 & -4 \\ 0 & 2 & 2 \\ 0 & 0 & 8 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 6 \\ 8 \end{bmatrix}$$

Starting at the bottom,

$8x_3 = 8 \Rightarrow x_3 = 1$

$2x_2 + 2(1) = 6 \Rightarrow x_2 = 2$

$4x_1 + 4(2) - 4(1) = 0 \Rightarrow x_1 = -1.$

Therefore, the solution is $x = [-1, 2, 1]$.

- **Partial Pivoting method**

- **Permutation Matrices**

- **PA= LU Factorization**


Thank
You
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