CHN-323
Computer Applications in Chemical Engineering

Ashwini Kumar Sharma

Department of Chemical Engineering
Indian Institute of Technology Roorkee
Email: ashwini.fch@iitr.ac.in

Set of equations

- Determine the values $x_1, x_2, x_3, \ldots, x_n$ that simultaneously satisfy a set of equations

$$
\begin{aligned}
f_1(x_1, x_2, \ldots, x_n) &= 0 \\
f_2(x_1, x_2, \ldots, x_n) &= 0 \\
&\vdots \\
f_n(x_1, x_2, \ldots, x_n) &= 0
\end{aligned}
$$

- Equations can be linear/nonlinear

Set of linear algebraic equations

$$
\begin{aligned}
&a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\
&a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\
&\vdots \\
&a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n = b_n
\end{aligned}
$$

- a's are constant coefficients
- b's are constants
- x's are unknowns
- n is the number of equations

Importance of linear equations

- Linear equations are the basis for mathematical models of
  - economics,
  - weather prediction,
  - heat and mass transfer,
  - statistical analysis, and
  - a myriad of other applications.
- The methods for solving ordinary and partial differential equations depend on them

Set of linear equations and matrix algebra

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$
$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2$$
$$\vdots$$
$$a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n = b_n$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$$AX = B$$

where $A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \quad X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \quad B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$

Matrix algebra

- Square matrix
- Symmetric matrix
- Diagonal matrix
- Identity matrix
- Upper triangular matrix
- Lower triangular matrix

Matrix algebra

- Matrix addition and subtraction
  - Commutative [A]+[B]= [B]+[A]
  - Associative ([A]+[B])+[C]= [A]+([B]+[C])

- Multiplication of a matrix with a scalar

- Multiplication of two matrices
  - Associative ([A][B]) [C]= [A] ([B][C])
  - Distributive ([A]([B]+[C])= [A][B]+ [A][C]
  - Not commutative [A][B]≠ [B][A]

Determinant of a matrix

$$[A] = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \qquad D = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$

$$|\mathrm{A}| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = (ad - bc)$$

$$|A| = \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a\begin{vmatrix} e & f \\ h & i \end{vmatrix} - b\begin{vmatrix} d & f \\ g & i \end{vmatrix} + c\begin{vmatrix} d & e \\ g & h \end{vmatrix}$$

$$= a(ei - fh) - b(di - fg) + c(dh - eg)$$

Solving linear equations in MATLAB

- $AX = B$

```
>> a=[1 2; 3, 4];
>> b=[3, 5];
>> b=b';
>> x=a\b

x =

    -1
     2
```

```
>> x=inv(A)*b
Unrecognized function or variable 'A'.

Did you mean:
>> x=inv(a)*b

x =

   -1.0000
    2.0000
```

Solving linear equation systems

- Three types of methods
  - Direct methods
  - Iterative methods
  - Decomposition methods

Solving linear equation systems

- A is a nxn matrix

$$[A][A]^{-1} = [A]^{-1}[A] = [I]$$

- Our system, $AX = B$
- Multiply both sides by A^{-1}

$$A^{-1}AX = A^{-1}B$$

$$X = A^{-1}B$$

$$A^{-1} = \frac{1}{|A|} \cdot \text{Adj } A$$

- Adj *A* means the adjoint matrix of *A*

- The adjoint of a matrix is the transpose of the cofactor element matrix of the given matrix.

Cramer's rule

- Our system $AX = B$
- Solution is given by

$$x_j = \frac{\det(A_j)}{\det(A)} \quad ; \det(A) \neq 0 \; ; \; j = 1, \cdots, n$$

- A_j is obtained by replacing the j^{th} column of A by B

Cramer's rule

- Total number of determinants required = $n+1$
- Number of operations to calculate determinant of a nxn matrix = $(n-1)\,(n!)$
- Total operations in Cramer's rule= $(n+1)\,(n-1)\,(n!)$

$$\sim n^2 n!$$

For a 100x100 matrix: $100^2\ 100! = 10^{162}$ calculations

Gauss elimination

- Consider the system

$$x_1+x_2+2x_3 = 3$$
$$2x_1+3x_2+x_3 = 2$$
$$3x_1-x_2-x_3 = 6$$

- Let us perform the following row operations

Old Eq (2) – 2 Eq (1) → New Eq (2): $x_2 - 3x_3 = -4$

Old Eq (3) – 3 Eq (1) → New Eq (3): $-4x_2 - 7x_3 = -3$

- The equivalent system of equations is

$$x_1+x_2+2x_3 = 3$$
$$x_2 -3x_3 = -4$$
$$-4x_2-7x_3 = -3$$

We have eliminated x_1 from Eq. (2) and (3).

Gauss elimination contd…

- Let us perform another elementary row operation

  Old Eq (3) + 4 Eq (2) → New Eq (3): $-19x_3 = -19$

- The new equivalent system of equations is

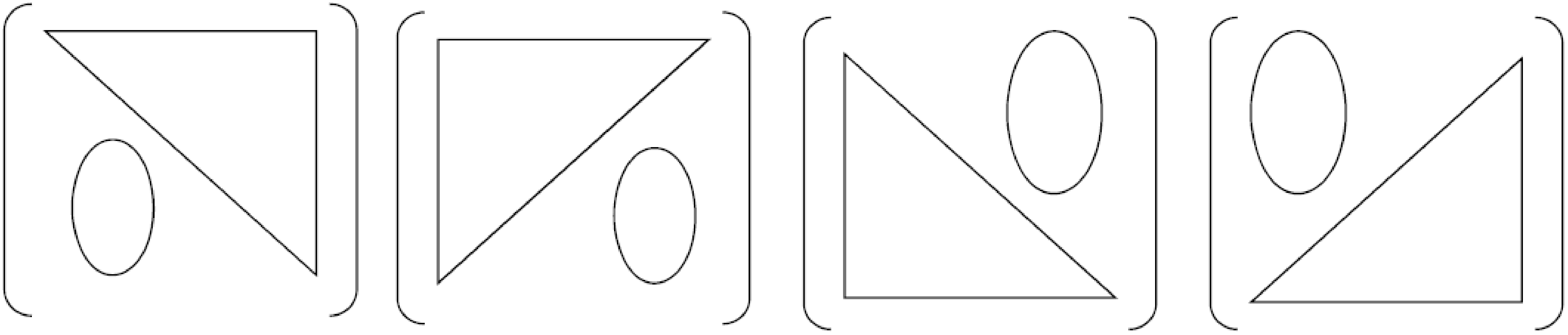
$$\begin{aligned} x_1 + x_2 + 2x_3 &= 3 \\ 0x_1 + x_2 - 3x_3 &= -4 \\ 0x_1 + 0x_2 - 19x_3 &= -19 \end{aligned}$$

We have eliminated x_2 from Eq. (3).

- Now, if we write in matrix format, the coefficient matrix is upper triangular matrix
  - That can be easily solved
  - Solve Eq. (3) to get $x_3=1$
  - Substitute $x_3=1$ in Eq. (2) to get $x_2= -1$
  - Substitute $x_3=1$ and $x_2= -1$ in Eq. (1) to get $x_1= 2$

Gauss elimination contd…

- Idea behind: Convert "full" coefficient matrix into a lower or upper triangular matrix (Note: the constant matrix on RHS will also be modified)



Upper Triangular Structure

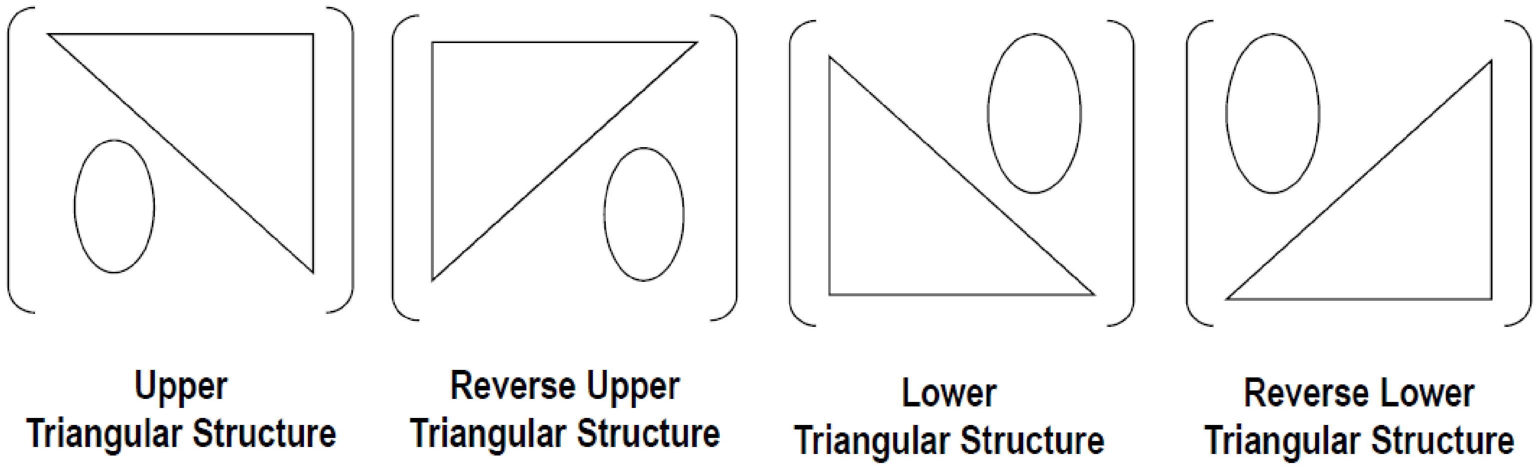
Reverse Upper Triangular Structure

Lower Triangular Structure

Reverse Lower Triangular Structure

Gauss elimination contd…

- If coefficient matrix is
  - Upper triangular, the system can be solved in sequence $x_n, x_{n-1}, \ldots, x_1$ using equations in order n, n-1, …, 1
  - Reverse upper triangular, the system can be solved in sequence $x_1, x_2, \ldots, x_n$ using equations in order n, n-1, …, 1
  - Lower triangular, the system can be solved in sequence $x_1, x_2, \ldots, x_n$ using equations in order 1, 2, …, n
  - Reverse lower triangular, the system can be solved in sequence $x_n, x_{n-1}, \ldots, x_1$ using equations in order 1, 2, …, n



Two stages of Gauss elimination

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & | & b_1 \\ a_{21} & a_{22} & a_{23} & | & b_2 \\ a_{31} & a_{32} & a_{33} & | & b_3 \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & | & b_1 \\ & a'_{22} & a'_{23} & | & b'_2 \\ & & a''_{33} & | & b''_3 \end{bmatrix}$$

(*a*) Forward elimination

$$\downarrow$$

$$x_3 = b''_3/a''_{33}$$

$$x_2 = (b'_2 - a'_{23}x_3)/a'_{22}$$

$$x_1 = (b_1 - a_{13}x_3 - a_{12}x_2)/a_{11}$$

(*b*) Back substitution

Forward elimination: generalization

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

- First, we eliminate x_1 from Eq. (2) and (3). To do so, we perform the following row operations

  New Eq (2) = Old Eq (2) – (a_{21}* Old Eq (1) / a_{11})

  New Eq (3) = Old Eq (3) – (a_{31}* Old Eq (1) / a_{11})

- a_{11} is the pivot element in the elimination of x_1 from Eq (2)&(3)

Forward elimination: generalization

- The new equivalent system is

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$\left(a_{22} - \left(\frac{a_{21}a_{12}}{a_{11}}\right)\right)x_2 + \left(a_{23} - \left(\frac{a_{21}a_{13}}{a_{11}}\right)\right)x_3 = b_2 - \frac{a_{21}b_1}{a_{11}}$$

$$\left(a_{32} - \left(\frac{a_{31}a_{12}}{a_{11}}\right)\right)x_2 + \left(a_{33} - \left(\frac{a_{31}a_{13}}{a_{11}}\right)\right)x_3 = b_3 - \frac{a_{31}b_1}{a_{11}}$$

- In other words,

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 = b'_2$$

$$a'_{32}x_2 + a'_{33}x_3 = b'_3$$

Diagonal elements are pivot elements

- Let us perform another elementary row operation

New Eq (3) = Old Eq (3) – (a'_{32} * Old Eq (2) / a'_{22})

$a'22$ is the pivot element in the elimination of x_2 from Eq (3)

Forward elimination: generalization

- The new equivalent system is

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 = b'_2$$

$$\left(a'_{33} - \left(\frac{a'_{32}a'_{23}}{a'_{22}}\right)\right)x_3 = b'_3 - \frac{a_{32}b_2}{a_{22}}$$

- In other words,

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$

$$a'_{22}x_2 + a'_{23}x_3 = b'_2$$

$$a''_{33}x_3 = b''_3$$

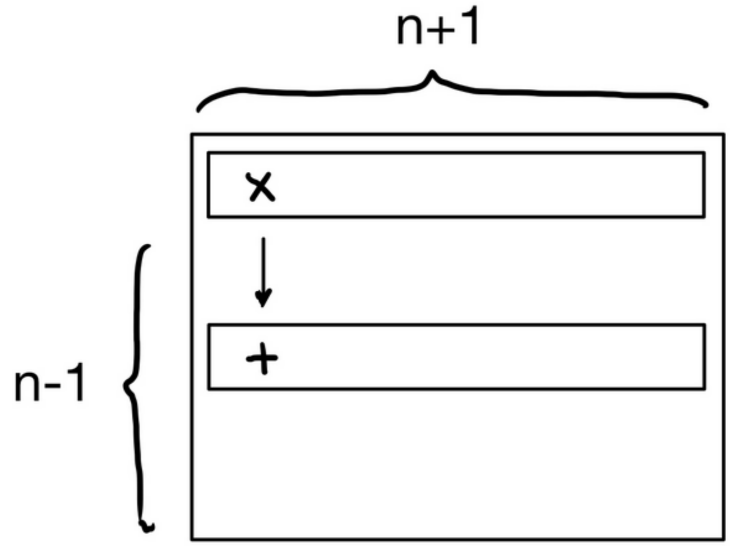
This is a upper triangular system and can be solved in sequential order x_3, x_2 and x_1

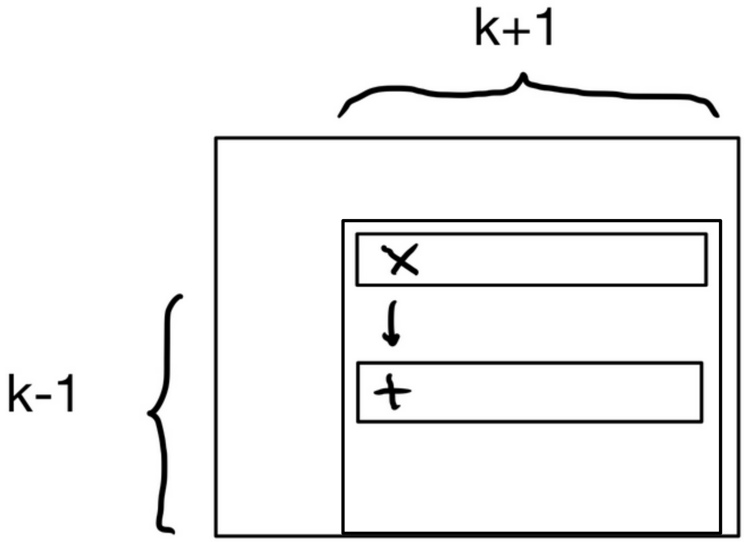
Forward elimination: Number of calculations

- For n equations in n unknowns, the augmented matrix is a nx(n+1) matrix.
- For each row i
  - Add a multiple of i^{th} row to all rows below it

New Eq (2) = Old Eq (2) – (a_{21}* Old Eq (1) / a_{11})

- For row 1, this process will require
  - There are (n-1) rows below row 1, each of those has (n+1) elements
  - Each element requires 1 multiplication, and 1 subtraction
  - Total calculations = 2 (n-1) (n+1) = $2n^2-2$
- When operating on i^{th} row, there are k = n-i+1 unknowns, so there are $2k^2-2$ calcs required





Forward elimination: Number of calculations

- k ranges from n down to 1
- So, the total number of arithmetic opns required

$$\sum_{k=1}^{n}(2k^2-2)=2\left(\sum_{k=1}^{n}k^2-\sum_{k=1}^{n}1\right)$$

$$=2\left(\frac{n(n+1)(2n+1)}{6}-n\right)$$

$$=\frac{2}{3}n^3+n^2-\frac{5}{3}n$$

Back-substitution: generalization

- Consider the system as Lx=b

$$\begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \ddots & 0 \\ \vdots & \vdots & \ddots & 0 \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

det (L) = $l_{11} * l_{22} * \cdots lnn = \prod_{i=1}^{n} l_{nn}$

For a non-singular L, all l_{ii} should be non-zero

Back-substitution: generalization

$$\begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \ddots & 0 \\ \vdots & \vdots & \ddots & 0 \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

$$l_{11}x_1 = b_1 \rightarrow x_1 = \frac{b_1}{l_{11}}$$

$$l_{21}x_1 + l_{22}x_2 = b_2 \rightarrow x_2 = \frac{b_2 - l_{21}x_1}{l_{22}}$$

And so on

$$l_{n1}x_1 + l_{n2}x_2 + \cdots + ln_{nxn} = bn \rightarrow$$

$$x_n = \frac{b_n - ln_1x_1 - l_{n2}x_2 - \cdots . - l_{n,n-1}x_{n-1}}{l_{nn}}$$

In general, $x_k = \dfrac{b_k - lk_1x_1 - l_{k2}x_2 - \cdots . - l_{k,k-1}x_{k-1}}{l_{kk}}$

Back-substitution: No. of calculations

$$x_1 = \frac{b_1}{l_{11}} \qquad x_2 = \frac{b_2 - l_{21}x_1}{l_{22}} \qquad x_k = \frac{b_k - lk_1x_1 - l_{k2}x_2 - \cdots . - l_{k,k-1}x_{k-1}}{l_{kk}}$$

To get x_1 $\rightarrow$ one division

To get x_2 $\rightarrow$ one division + one subtraction + one multiplication

To get x_3 $\rightarrow$ one division + two subtractions + two multiplications

….

To get x_n $\rightarrow$ one division + (n-1) subtractions + (n-1) multiplications

Total calculations to get $x_1, x_2, \ldots, x_n$ $\rightarrow$

n divisions + (1+2+…+(n-1)) subtractions + (1+2+…+(n-1) multiplications

i.e., approximately n^2 calculations

Gauss elimination: with matrix format

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} \vdots & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \end{bmatrix}$$

Augmented matrix

$$\begin{bmatrix} 1 & 1 & 2 & 3 \\ 2 & 3 & 1 & \vdots\, 2 \\ 3 & -1 & -1 & 6 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 1 & 2 & 3 \\ 0 & 1 & -3 & \vdots\, -4 \\ 0 & -4 & -7 & -3 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 1 & 2 & 3 \\ 0 & 1 & -3 & \vdots\, -4 \\ 0 & 0 & -19 & -19 \end{bmatrix}$$

$$\rightarrow \quad x = \begin{bmatrix} 2 \\ -1 \\ 1 \end{bmatrix}$$

Example: linearly dependent system

$$\begin{bmatrix} 1 & 2 & -1 & -2 & -1 \\ 2 & 1 & 1 & -1 & 4 \\ 1 & -1 & 2 & 1 & 5 \\ 1 & 3 & -2 & -3 & -3 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 2 & -1 & -2 & -1 \\ 0 & -3 & 3 & 3 & 6 \\ 0 & -3 & 3 & 3 & 6 \\ 0 & 1 & -1 & -1 & -2 \end{bmatrix}$$

The **rank** of a matrix is defined as (a) the maximum number of linearly independent *row* vectors in the matrix or (b) the maximum number of linearly independent *column* vectors in the matrix.

Rank of augment matrix = rank of coefficient matrix = 2

Number of unknowns = 4

Example: pivot element is zero

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

a_{11} = 0, cannot be used for pivoting

Perform row interchange. Interchange rows (1) and (2)

$$A = \begin{bmatrix} 1 & 1 & 2 \\ 0 & 1 & 1 \\ 4 & 5 & 6 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 & 2 \\ 0 & 1 & 1 \\ 0 & 1 & -2 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 & 2 \\ 0 & 1 & 1 \\ 0 & 0 & -3 \end{bmatrix}$$

Coefficient Matrix is Upper Triangular

Rule: If pivot element = 0, then interchange that row with any of the later rows which will have a non-zero pivot element.

Example: pivot element is too small

- Sometimes, the candidate pivot element is quite small but not zero. Though, this does not lead to the "mathematical breakdown" of the algorithm, it does have a detrimental effect on the quality of the obtained solution when implemented on a finite precision computer.

$$\begin{bmatrix} 0.0001 & 0.5 \\ 0.4 & -0.3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.1 \end{bmatrix}$$

Our PC does 4-digit rounded decimal arithmetic

$$\left[\begin{array}{cc|c} 0.0001 & 0.5 & 0.5 \\ 0.4 & -0.3 & 0.1 \end{array}\right] \Rightarrow \left[\begin{array}{cc|c} 1 & 5000 & 5000 \\ 0 & -2000 & -2000 \end{array}\right]$$

Rounded value of -2000.3

Rounded value of -1999.9

$x_1 = 0$
$x_2 = 1$

Wrong Solution

Rule: Avoid not only "zero" for the pivot element but also small pivots.

Pivoting

- Partial Pivoting: Make the element that is largest in magnitude from the remaining rows as the pivot element
- Threshold Pivoting: Perform interchange of rows only if the natural pivot element is significantly smaller than the competitor
- Complete Pivoting: Largest element in the entire remaining matrix is made the pivot element. This strategy therefore involves interchange of both rows and columns.