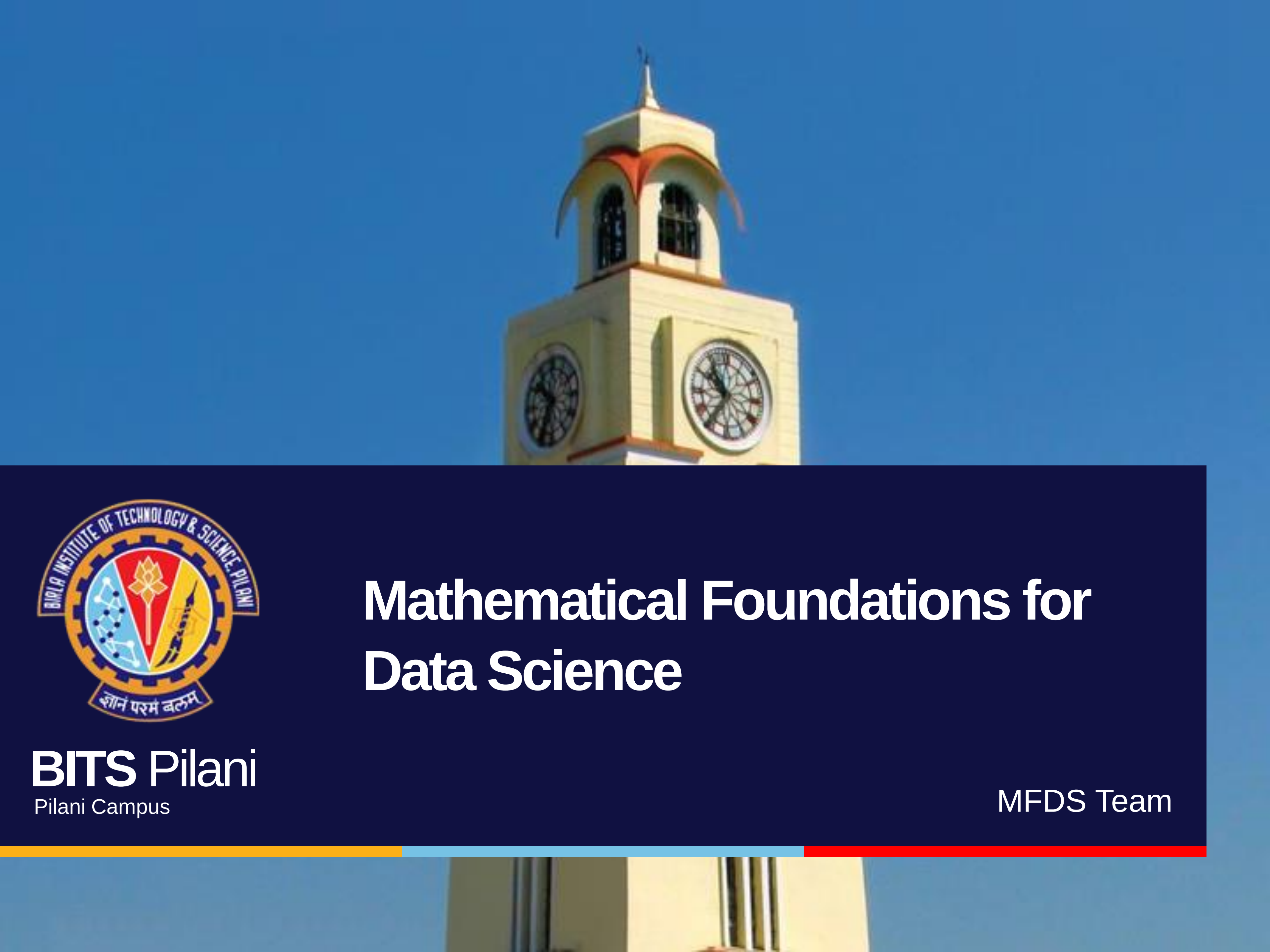

Mathematical Foundations for Data Science

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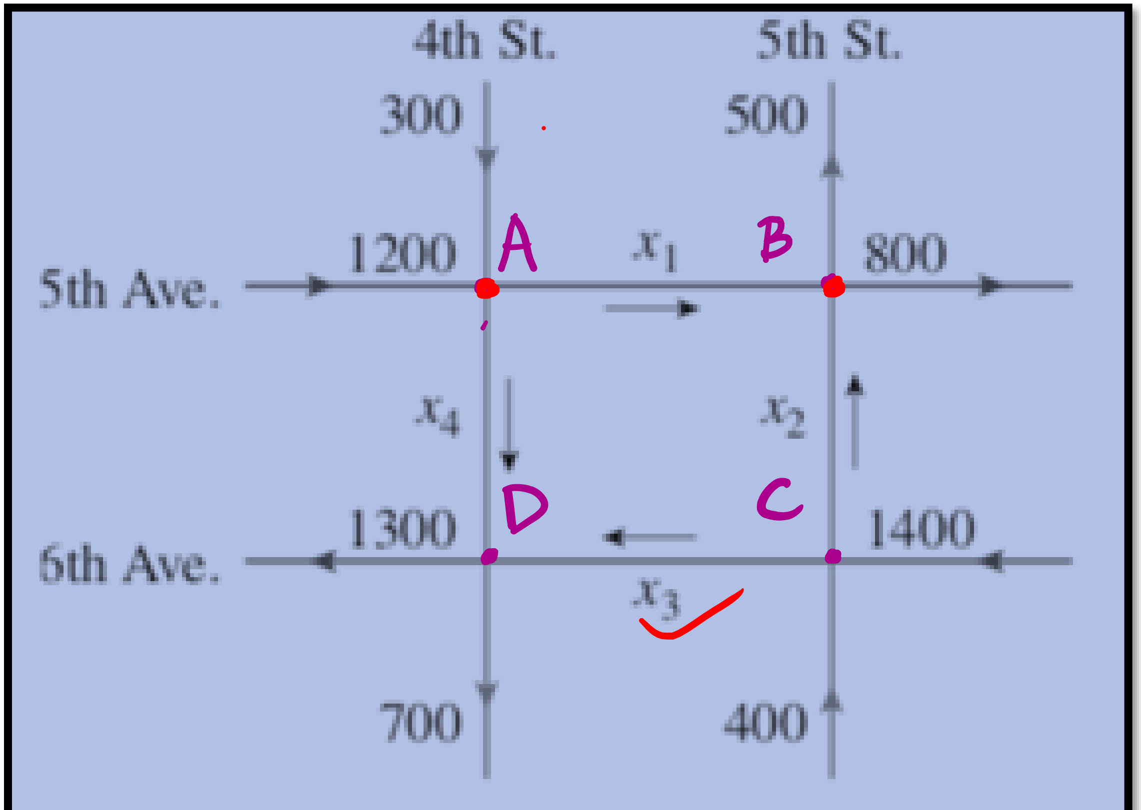
Lecture No.1

Agenda

- Application of Linear Algebra : Traffic Flow
- Norms of vectors
- Linear Systems
- Augmented Matrices and Linear Systems
  - Gaussian Elimination using matrices
- Consistent and Inconsistent linear Systems
  - Consistent : Unique Solution and Infinite Solution
- Pitfalls in Gaussian Elimination
  - Gaussian Elimination with Partial Pivoting
- LU factorization of a matrix
  - LU factorization and Linear Systems

Linear Equations in Traffic Flow Problem

Traffic Flow



	Junction
$x_1 + x_4 = 1500$	A
$x_1 + x_2 = 1300$	B
$x_2 + x_3 = 1800$	C
$x_3 + x_4 = 2000$	D

$$0x_1 + 0x_2 + 1x_3 + 1\cdot x_4 = 2000$$

$$\left[\begin{array}{cccc|c} 1 & 0 & 0 & 1 & 1500 \\ 1 & 1 & 0 & 0 & 1300 \\ 0 & 1 & 1 & 0 & 1800 \\ 0 & 0 & 1 & 1 & 2000 \end{array}\right]$$

Norms of Vectors

$$x = \begin{bmatrix} 1 \\ 2 \\ -3 \end{bmatrix} \qquad \|x\|_2 = \sqrt{1^2 + 2^2 + (-3)^2}$$

a) l_1 norm $\quad \|x\|_1 = |1| + |2| + |-3| = 6$

b) l_2 norm $\quad \|x\|_2 = \sqrt{|1|^2 + |2|^2 + |-3|^2} = 14$

c) l_∞ norm $\quad \|x\|_\infty = \max\{|1|, |2|, |-3|\}$

$$= \max\{1, 2, 3\} = 3$$

Norms

Norm – A norm is a function f(x)= $||x||$ that takes as input a vector .
In addition it has the following 4 properties :

1. $||x|| \geq 0$
2. $||x||=0$ if and only if x=0
3. $||cx|| = |c|\ ||x||$ where c is some constant
4. $||x + y|| \leq ||x|| + ||y||$

$x = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ $y = \begin{bmatrix} 2 \\ -3 \end{bmatrix}$

1. $\left\|\begin{bmatrix} 1 \\ 2 \end{bmatrix}\right\|_1 = |1| + |2| = 3$ $\left\|\begin{bmatrix} 2 \\ -3 \end{bmatrix}\right\|_1 = |2| + |-3| = 5$

3. $||2x|| = \left\|\begin{bmatrix} 2 \\ 4 \end{bmatrix}\right\| = 6$ $2\left\|\begin{bmatrix} 1 \\ 2 \end{bmatrix}\right\|_1 = 2\,(|1| + |2|) = 6$

4 $\left\|\begin{bmatrix} 3 \\ -1 \end{bmatrix}\right\|_1 = 4 \leq ||x||_1 + ||y||_1$

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Solve the Linear System

$$2x + y = 7 \rightarrow ①$$
$$x - y = -1 \rightarrow ②$$

$$\begin{bmatrix} 2 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 7 \\ -1 \end{bmatrix}$$

$$\text{Eq}② - \tfrac{1}{2}\,\text{Eq}(1) \Rightarrow 0x - \tfrac{3}{2}y = -\tfrac{9}{2}$$

$$2x + y = 7$$
$$0x - \tfrac{3}{2}y = -\tfrac{9}{2}$$

$$\begin{bmatrix} 2 & 1 \\ 0 & -3/2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 7 \\ -9/2 \end{bmatrix}$$

Step 1

$$-\tfrac{3}{2}y = -\tfrac{9}{2} \Rightarrow y = 3$$

$$2x + 3 = 7 \Rightarrow x = 2$$

Step 2

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Augmented Matrix of $Ax=b$

$$\left[\begin{array}{cc|c} 2^{a_{11}} & 1 & 7 \\ 1^{a_{21}} & -1 & -1 \end{array}\right] \xrightarrow{R_2 \leftarrow R_2 - \frac{1}{2}R_1} \left[\begin{array}{cc|c} \boxed{2} & 1 & 7 \\ 0 & \boxed{\frac{-3}{2}} & \frac{-9}{2} \end{array}\right]$$

Step 1

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n eqns

n unknowns

Linear Eqn Form $\longrightarrow$ $\underbrace{Ax = b}_{\text{Matrix Form}}$ -

$$
\begin{aligned}
E_1: \quad & a_{11}x_1 + \cdots + a_{1n}x_n = b_1 \\
E_2: \quad & a_{21}x_1 + \cdots + a_{2n}x_n = b_2 \\
& \cdots\cdots\cdots\cdots\cdots\cdots \\
E_n: \quad & a_{n1}x_1 + \cdots + a_{nn}x_n = b_n
\end{aligned}
$$

$$
\overbrace{\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & & a_{2n} \\ a_{n1} & a_{n2} & & a_{nn} \end{bmatrix}}^{A} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}
$$

Matrix Form of the Linear System

From the definition of matrix multiplication we see that the m equations of (1) may be written as a single vector equation

(2) $\mathbf{Ax} = \mathbf{b}$ n x n

where the **coefficient matrix A** = $[a_{jk}]$ is the $m \times n$ matrix

n

$$\mathbf{A} = \underbrace{\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdot & \cdot & \cdots & \cdot \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}}_{m}, \quad \text{and} \quad \mathbf{x} = \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} \Big\} n \quad \text{and} \quad \mathbf{b} = m \Big\{ \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$

are column vectors.

Augmented Matrix

Matrix Form of the Linear System (1). (continued)

We assume that the coefficients a_{jk} are not all zero, so that **A** is not a zero matrix. Note that **x** has n components, whereas **b** has m components. The matrix

(n+1)

$$m \quad \tilde{\mathbf{A}} = \left[\begin{array}{ccc|c} a_{11} & \cdots & a_{1n} & b_1 \\ \cdot & \cdots & \cdot & \cdot \\ \cdot & \cdots & \cdot & \cdot \\ a_{m1} & \cdots & a_{mn} & b_m \end{array}\right]$$

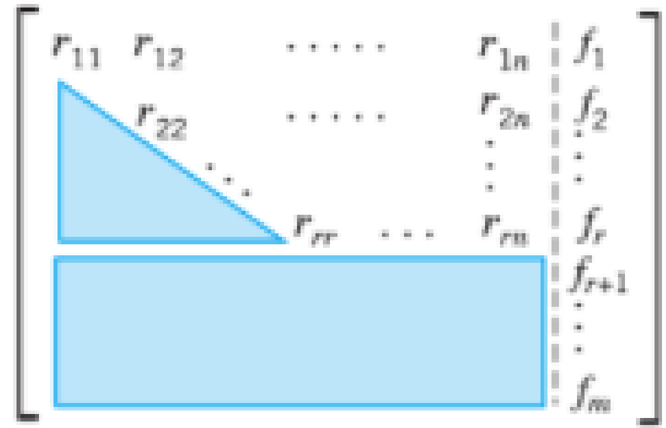
m eqns
n unknowns

$A_{m \times n}$

is called the **augmented matrix** of the system (1). The dashed vertical line could be omitted, as we shall do later. It is merely a reminder that the last column of $\tilde{\mathbf{A}}$ did not come from matrix **A** but came from vector **b**. Thus, we *augmented* the matrix **A**.

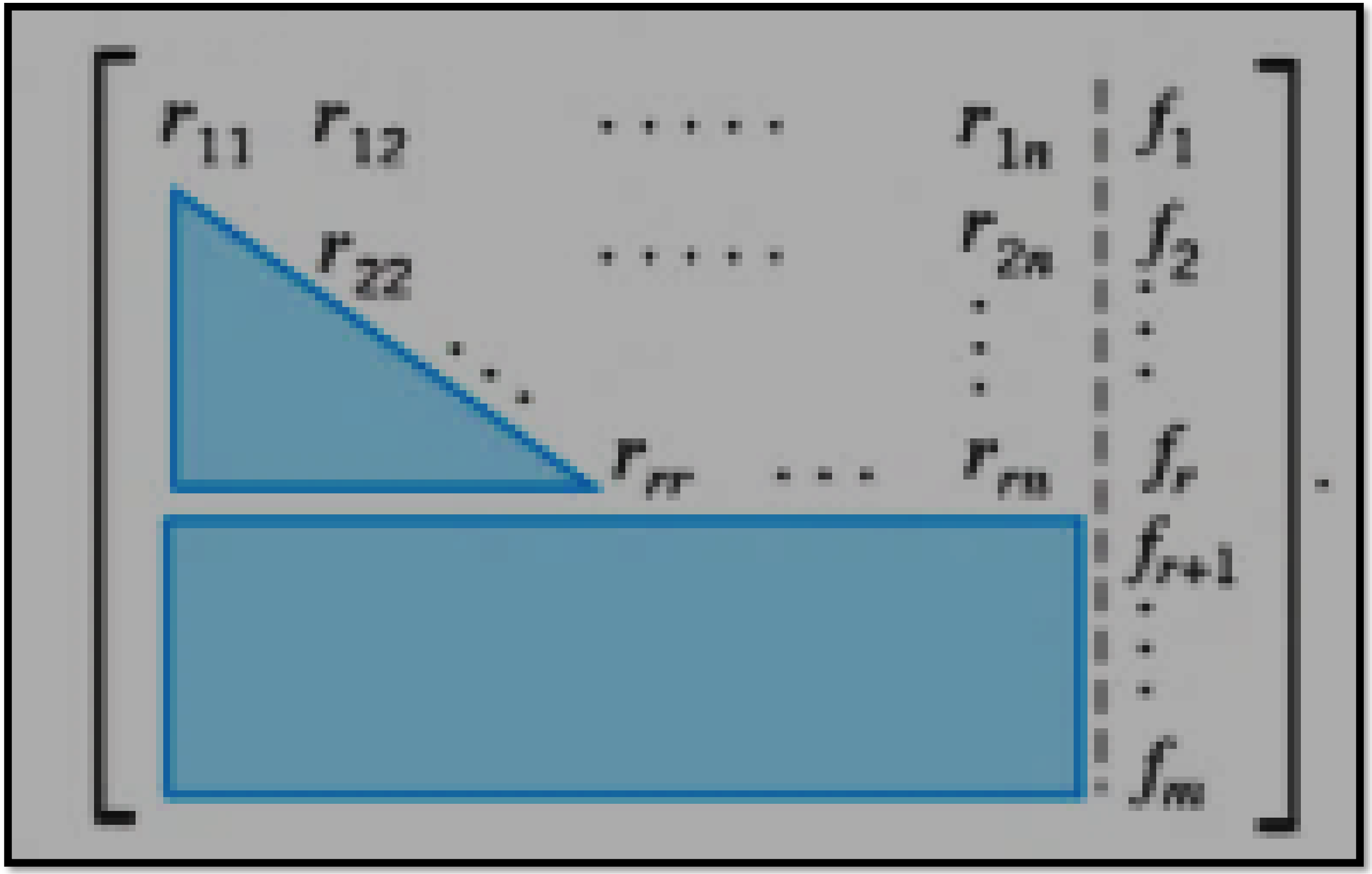
Gauss Elimination

At the end of the Gauss elimination (before the back substitution), the row echelon form of the augmented matrix will be



1. in upper triangular form
2. have the first r (r is rank) rows non-zero
3. Exactly m - r rows would be zero rows
4. If consistent , then last m- r rows will be zero rows
5. If any one of the last m-r rows is non-zero, it would imply inconsistency
6. facilitates the back substitution

Gauss Elimination : convert [A |b] to REF



Case 1 : Inconsistent Linear System
Case 2 : Consistent Linear System

❑ Inconsistent (No solution)

If r is less than m (meaning that **R** actually has at least one row of all 0s) *and* at least one of the numbers $f_{r+1}, f_{r+2}, \ldots, f_m$ is not zero, then the system $\mathbf{Rx} = \mathbf{f}$ is inconsistent. Therefore the system $\mathbf{Ax} = \mathbf{b}$ is inconsistent as well.

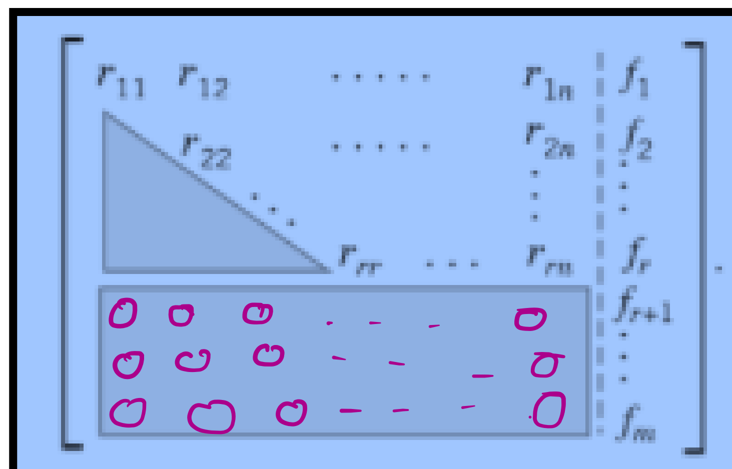
❑ Consistent (Atleast one solution)

- Otherwise : Ax=b is consistent

1. Find ref([A|b])

2) If there is a row where only f column is nonzero, then Ax=b is inconsistent

3. Consistent otherwise



Inconsistent Linear System

$$\boxed{\begin{aligned} x_1 + x_2 &= 1 \\ x_1 + x_2 &= 0 \end{aligned}}$$

$$\left[\begin{array}{cc|c} 1 & 1 & 1 \\ 1 & 1 & 0 \end{array}\right] \xrightarrow{R_2 \leftarrow R_2 - R_1} \begin{array}{c} \begin{array}{cc|c} R & & f \end{array} \\ \left[\begin{array}{cc|c} 1 & 1 & 1 \\ 0 & 0 & -1 \end{array}\right] \end{array}$$

HW: $x_1 + x_2 = 1$

$2x_1 + 2x_2 = 0$

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"Consistent Linear System"

$$x_1 + x_2 = 1$$
$$x_1 - x_2 = 2$$

Consistent

$$\tilde{A} = \left[\begin{array}{cc|c} 1 & 1 & 1 \\ 1 & -1 & 2 \end{array}\right] \xrightarrow{R_2 \leftarrow R_2 - R_1} \left[\begin{array}{cc|c} 1 & 1 & 1 \\ 0 & -2 & 1 \end{array}\right]$$

$$-2x_2 = 1 \Rightarrow x_2 = -0.5$$

$$x_1 = 1 - x_2 = 1.5$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1.5 \\ -0.5 \end{bmatrix}$$

HW: $2x_1 + x_2 = 7$
$3x_1 + 2x_2 = 5$

Pitfalls of Gauss Elimination

Problem 1 : Division by zero

It is possible that during both elimination and back-substitution phases a division by zero can occur.

For example:

$$
\begin{aligned}
2x_2 + 3x_3 &= 8 \\
4x_1 + 6x_2 + 7x_3 &= -3 \\
2x_1 + x_2 + 6x_3 &= 5
\end{aligned}
\qquad
A = \begin{matrix} 0 & 2 & 3 \\ 4 & 6 & 7 \\ 2 & 1 & 6 \end{matrix}
$$

$a_{11} = 0$
(the pivot element)

Solution: Partial **Pivoting**

Pitfalls of Gauss Elimination

Problem 2 : Roundoff Errors

1. Because computers carry only a limited number of significant figures, round-off errors will occur and they will *propagate* from one iteration to the next.

2. This problem is especially important when **large** numbers of equations (100 or more) are to be solved.

Order 1

$$0.4003\ x_1 - 1.502\ x_2 = 2.501$$
$$0.0004\ x1 + 1.402\ x_2 = 1.406$$

Order 2

$$0.0004\ x1 + 1.402\ x_2 = 1.406$$
$$0.4003\ x_1 - 1.502\ x_2 = 2.501$$

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Gauss Elimination : Rounding with 4 significant digits

Order 1

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$$m = \frac{a_{21}}{a_{11}}$$

$$\begin{bmatrix} 0.4003 & -1.502 & 2.501 \\ 0.0004 & 1.402 & 1.406 \end{bmatrix} \xrightarrow[R_2 \leftarrow R_2 - mR_1]{} \begin{bmatrix} 0.4003 & -1.502 & 2.501 \\ 0 & 1.404 & 1.404 \end{bmatrix}$$

REF

Note $m = \frac{0.0004}{0.4003} = 0.000999251 \longrightarrow 0.0009993$

$1.404x_2 = 1.404 \Rightarrow x_2 = 1$

In ① substitute $x_2 = 1$, $\Rightarrow x_1 = 10$.

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Gauss Elimination : Rounding with 4 significant digits

Order 2

$$\begin{bmatrix} 0.0004 & 1.402 & 1.406 \\ 0.4003 & -1.502 & 2.501 \end{bmatrix} \xrightarrow{R_2 \leftarrow R_2 - mR_1} \begin{bmatrix} 0.0004 & 1.402 & 1.406 \\ 0 & -1405 & -1404 \end{bmatrix}$$

$$m = \frac{0.4003}{0.0004} = 1000.75 \simeq 1001$$

$$-1.405\, x_2 = -1.404 \implies x_2 = 0.99928 = 0.9993$$

$$0.0004\, x_1 = 0.005$$

$$\implies x_1 = 12.5$$

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Techniques for Improving the solution

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Use of more significant figures – double precision arithmetic

1. Pivoting

If a pivot element is zero, normalization step leads to division by zero. The same problem may arise, when the pivot element is close to zero.

- ***Partial pivoting***

  Switching the rows below so that the largest element is the pivot element.

- ***Complete pivoting***

2. Scaling

-

Partial Pivoting – Example 2

Pivoting Example

Example 14: Solve the following system using Gauss Elimination with pivoting.

$$
\begin{aligned}
2x_2 + + x_4 &= 0 \\
2x_1 + 2x_2 + 3x_3 + 2x_4 &= -2 \\
4x_1 - 3x_2 + x_4 &= -7 \\
6x_1 + x_2 - 6x_3 - 5x_4 &= 6
\end{aligned}
$$

Step 0: Form the augmented matrix

$$
\left[\begin{array}{cccc|c}
0 & 2 & 0 & 1 & 0 \\
2 & 2 & 3 & 2 & -2 \\
4 & -3 & 0 & 1 & -7 \\
6 & 1 & -6 & -5 & 6
\end{array}\right]
$$

Step 1: Forward Elimination

(1.1) Eliminate x_1 . But the pivot element is 0. We have to interchange the 1st row with one of the rows below it. Interchange it with the 4th row because 6 is the largest possible pivot.

(1.1) Eliminate x_1 . But the pivot element is 0. We have to interchange the 1st row with one of the rows below it. Interchange it with the 4th row because 6 is the largest possible pivot.

$$
\left[\begin{array}{cccc|c}
6 & 1 & -6 & -5 & 6 \\
2 & 2 & 3 & 2 & -2 \\
4 & -3 & 0 & 1 & -7 \\
0 & 2 & 0 & 1 & 0
\end{array}\right]
$$

Now eliminate x_1

$$
\left[\begin{array}{cccc|c}
6 & 1 & -6 & -5 & 6 \\
0 & 1.6667 & 5 & 3.6667 & -4 \\
0 & -3.6667 & 4 & 4.3333 & -11 \\
0 & 2 & 0 & 1 & 0
\end{array}\right]
$$

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Partial Pivoting – Example 2

(1.2) Eliminate x_2 .from the 3rd and 4th eqns. Pivot element is 1.6667. There is no division by zero problem. Still we will perform pivoting to reduce round-off errors. Interchange the 2nd and 3rd rows. Note that complete pivoting would interchange 2nd and 3rd columns.

6	1	-6	-5	|	6
0	-3.6667	4	4.3333	|	-11
0	1.6667	5	3.6667	|	-4
0	2	0	1	|	0

Eliminate x_2

6	1	-6	-5	|	6
0	-3.6667	4	4.3333	|	-11
0	0	6.8182	5.6364	|	-9.0001
0	0	2.1818	3.3636	|	-5.9999

(1.3) Eliminate x_3 . 6.8182 > 2.1818, therefore no pivoting is necessary.

6	1	-6	-5	|	6
0	-3.6667	4	4.3333	|	-11
0	0	6.8182	5.6364	|	-9.0001
0	0	0	1.5600	|	-3.1199

Step 2: Back substitution

x_4 = -3.1199 / 1.5600 = **-1.9999**

x_3 = [-9.0001 – 5.6364*(-1.9999)] / 6.8182 = **0.33325**

x_2 = [-11 – 4.3333*(-1.9999) – 4*0.33325] / -3.6667 = **1.0000**

x_1 = [6 – (-5)*(-1.9999) – (-6)*0.33325 – 1*1.0000] / 6 = **-0.50000**

Exact solution is $x = [-2 \quad 1/3 \quad 1 \quad -0.5]^T$. Use more than 5 sig. figs. to reduce round-off errors.

Operation Count – Gauss Elimination

Important factors in judging the quality of a numerical method are

- Amount of storage
- Amount of time (= number of operations)

Consider Augmented Matrix of Ax = b, where $a_{in+1} = b_i$

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n+1} \\ a_{21} & a_{22} & \dots & a_{2n+1} \\ \vdots & & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn+1} \end{bmatrix}$$

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$$
\begin{array}{cc}
 & \begin{array}{cc} 1 & \overbrace{\qquad\qquad\qquad}^{n \text{ entries}} \end{array} \\
n & \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n+1} \\ a_{21} & a_{22} & \cdots & a_{2n+1} \\ \vdots & & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn+1} \end{bmatrix}
\end{array}
$$

1) Step1 : Find multiplier m to multiply row 1 with

2) Step2 : $R_2 \leftarrow R_2 + mR_1$

$m = \frac{a_{21}}{a_{11}}$

mR_1

$R_2 \leftarrow R_2 - mR_1$

a) No of divisions = $\boxed{1}$

b) No of multiplications = $\boxed{n}$

c) No of subtractions = $\boxed{n}$

$$\begin{array}{c} \text{n entries} \\ \left.\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n+1} \\ a_{21} & a_{22} & \cdots & a_{2n+1} \\ \vdots & \ddots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn+1} \end{bmatrix}\right\} n-1 \end{array}$$

a) No of divisions = $\boxed{1} * (n-1)$

b) No of multiplications = $\boxed{n} * (n-1)$

c) No of subtractions = $\boxed{n} * (n-1)$

Pivot No	Division	Multi	Subtraction
1	$1*(n-1)$	$n*(n-1)$	$n*(n-1)$
2	$1*(n-2)$	$(n-1)*(n-2)$	$(n-1)*(n-2)$
3	$1*(n-3)$	$(n-2)*(n-3)$	$(n-2)*(n-3)$
4			
5			
6			
k	$1*(n-k)$	$(n-k)(n-k+1)$	$(n-k)*(n-k+1)$

Operation Count – Gauss Elimination

Total number of multiplications and additions $2.\sum_{k=1}^{n-1}(n-k)(n-k+1)=O(n^3)$

Total number of divisions is $\sum_{k=1}^{n-1}(n-k)=O(n^2)$

$$f(n)=\sum_{k=1}^{n-1}(n-k)+2\sum_{k=1}^{n-1}(n-k)(n-k+1) \qquad (\text{write } n-k=s)$$

$$=\sum_{s=1}^{n-1}s+2\sum_{s=1}^{n-1}s(s+1)=\tfrac{1}{2}(n-1)n+\tfrac{2}{3}(n^2-1)n\approx\tfrac{2}{3}n^3$$

In back substitution total number of additions, multiplications and divisions required are

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

Algorithm	$n = 1000$	$n = 10000$
Elimination	0.7 sec	11 min
Back substitution	0.001 sec	0.1 sec

If an operation takes 10^{-9} sec, then

Back Substitution Operations

Consider

$k=1$ $\quad 5x_1+7x_2+3x_3+5x_4=10 \longrightarrow$ 1 div 3 sub 3 mult

$k=2$ $\quad 9x_2+2x_3+2x_4=7 \longrightarrow$ 1 div, 2 sub, 2 mult

$k=3$ $\quad 3x_3+2x_4=8 \longrightarrow$ 1 div, 1 sub 1 mult

$k=4$ $\quad 5x_4=11 \longrightarrow$ 1 div, 0 sub, 0 mult

In general for k^{th} equation

1 division, $n-k$ sub, $n-k$ multiplication

Total = n div, $\sum_{k=1}^{n}(n-k)$ sub, $\sum_{k=1}^{n}(n-k)$ mult

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