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#### Computers & Numerical Analysis (STR 681)

# Introduction

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# Why Do We Need Numerical Analysis Methods?



- Numerical methods are techniques by which mathematical problems are formulated so that they can be solved with arithmetic operations.

All numerical methods involves large numbers of arithmetic calculations.



- There are three approaches for problem solving using non-computer methods.
  - ✓ Analytical (Exact Approach).
  - ✓ Graphical Solution.
  - ✓ Calculators and Slide Rules.



- 1. Analytical (exact approach):
  - Excellent insight into behavior.
  - Derived for only a limited class of problems.
  - Approximated for linear models, simple geometry, and low dimensionality.
  - Limited practical value
  - Real problems are nonlinear, complex, in shape and processes.

- 2. Graphical solutions:
  - > Characterize the behavior of systems.
  - Used to solve complex problems.
  - Not very precise.
  - Extremely tedious and awkward to implement.



3. Calculators and Slide Rules:

> Implement numerical methods manually.

>Adequate for solving complex solutions.

➢ But slow and tedious.

Consistency results are elusive: blunders.



Computers and numerical methods provide an alternative method for such calculations.

Using computer power, problems can be approached without large simplifications or time-intense techniques.

# Acknowledgement

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#### PRESENTATION

# **Course Outline**



# Regulations



إنش ٦٨١: الحاسب والتحليل عددي

مقدمة: البرمجة، حل المسائل، الخوارزميات، خريطة الانسياب، مقدمة عن التحليل الرقمى باستخدام الحاسب، تحليل الخطأ: أخطاء التمثيل والقطع والتقريب، المجموعات الخطية من المعادلات الجبرية: مشاكل الصفرية وسوء الضبط والدقة، طرق الإزالة: طرق حل المصفوفات الشريحية المتماثلة، مسألة القيم الذاتية: طريق الأس، طريقة جاكوبس، الطريقة المباشرة.

#### STR681 Computer and Numerical Analysis

Introduction: programming, problem solving, algorithm, flowcharting; Introduction to computer based numerical analysis; Error analysis: modeling, truncation, and round off errors; Linear sets of algebraic equations: singularity, ill-conditioning, and accuracy; Elimination techniques: banded and symmetric solvers, Eigen value problem: power method, Jacobi method, direct method.

- □ Systems of Linear Algebraic Equations
- Nonlinear Equations
- Polynomial Approximation & Interpolation
- Numerical Differentiation & Difference
   Formulas
- Numerical Integration
- Discretization & Finite Difference Methods

- Weighted Residual Approach
- D Piecewise Functions
- □ Finite Element Methods
- **Optimization**
- **G** Curve Fitting
- Ordinary Differential Equations
- Partial Differential Equations



- Perturbation methods
- □ Fourier analysis
- □ Approximations & Round-off Errors



# Programming Language

MATLAB Program

# **Grading System**





# Systems of Linear Algebraic Equations

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = 0$$
  

$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = 0$$
  

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad \vdots$$
  

$$a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n = 0$$

# Systems of Linear Algebraic Equations

□ Systems of linear algebraic equations:

These problems are concerned with the value of a set of variables that satisfies a set of linear equations.

Given the a's and the c's, solve  $a_{11}x_1 + a_{12}x_2 = c_1$   $a_{21}x_1 + a_{22}x_2 = c_2$ for the x's.



## Systems of Linear Algebraic Equations

$$a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1$$
  
$$a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2$$

 $a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n$ 



 $[A]{X} = {B}$ 





 $[B] = [b_1 \quad b_2 \quad \cdots \quad b_m]$ Row vector, n = 1 $[C] = \begin{bmatrix} c_1 \\ c_2 \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$ Column vector, m = 1 $\Gamma_{a_{11}}$   $a_{12}$   $a_{13}$ Sq

quare matrix, n = m 
$$[A] = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

Symmetric matrix

$$[A] = \begin{bmatrix} 3 & 1 & 2 \\ 1 & 3 & 7 \\ 2 & 7 & 8 \end{bmatrix}$$

1

27

**Г** 5

$$a_{ij} = a_{ji}$$

Diagonal matrix  $[A] = \begin{bmatrix} a_{11} & & & \\ & a_{22} & & \\ & & a_{33} & \\ & & & a_{44} \end{bmatrix} \begin{bmatrix} 2 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ Identity matrix  $[I] = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ 

Upper triangular  $[A] = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ & a_{22} & a_{23} & a_{24} \\ & & & a_{33} & a_{34} \end{bmatrix} \begin{bmatrix} 1 & 4 & 3 \\ 0 & 8 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ 6 9  $a_{44}$ 0 Lower triangular matrix  $\begin{bmatrix} A \end{bmatrix} = \begin{bmatrix} a_{11} & & & & \\ a_{21} & a_{22} & & & \\ a_{31} & a_{32} & a_{33} & \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} 5 & 8 & 0 & 0 \\ 7 & 2 & 1 & 0 \\ 2 & 7 & 6 & 11 \end{bmatrix}$  $[A] = \begin{bmatrix} a_{11} & a_{12} & & & \\ a_{21} & a_{22} & a_{23} & & \\ & a_{32} & a_{33} & a_{34} & & \\ & & a_{43} & a_{44} & & \\ \end{bmatrix} \begin{bmatrix} 5 & 8 & 3 & \\ 0 & 2 & 1 & \\ 0 & 0 & 6 & \\ \end{bmatrix} \begin{bmatrix} 0 & 2 & 1 & \\ 0 & 0 & 6 & \\ \end{bmatrix}$ () Banded matrix Ex., Band width = 3(tridiagonal matrix)

[A] = [B] if  $a_{ij} = b_{ij}$  for all *i* and *j*.



[A] + [B] : $c_{ij} = a_{ij} + b_{ij}$ 

$$\begin{bmatrix} 1 & 4 \\ 2 & 6 \end{bmatrix} + \begin{bmatrix} 2 & 8 \\ 0 & 9 \end{bmatrix} = \begin{bmatrix} 3 & 12 \\ 2 & 15 \end{bmatrix}$$

$$d_{ij} = e_{ij} - f_{ij}$$

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



([A] + [B]) + [C] = [A] + ([B] + [C])



$$[D] = g[A] = \begin{bmatrix} ga_{11} & ga_{12} & \cdots & ga_{1m} \\ ga_{21} & ga_{22} & \cdots & ga_{2m} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ ga_{n1} & ga_{n2} & \cdots & ga_{nm} \end{bmatrix}$$

$$2x\begin{bmatrix} 1 & 4 & 5 \\ 7 & 12 & 2 \\ 8 & 3 & 4 \end{bmatrix} = \begin{bmatrix} 2 & 8 & 10 \\ 14 & 24 & 4 \\ 16 & 6 & 8 \end{bmatrix}$$

#### [C] = [A][B]

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

[*A*] is an *n* by *m* matrix, [*B*] could be an *m* by *I* matrix column row

[A][B] = [C]







([A][B])[C] = [A]([B][C])

[A]([B] + [C]) = [A][B] + [A][C]

# ([A] + [B])[C] = [A][C] + [B][C]

 $[A][B] \neq [B][A]$ 

If A is a square matrix:  $[A][A]^{-1} = [A]^{-1}[A] = [I]$ 

A<sup>-1</sup> is the inverse of A

$$[A]^{-1} = \frac{1}{a_{11}a_{22} - a_{12}a_{21}} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$$
  
Ex., A = 
$$\begin{bmatrix} 5 & 9 \\ 7 & 2 \end{bmatrix} \longrightarrow A^{-1} = \frac{1}{5x2 - 9x7} \begin{bmatrix} 2 & -9 \\ -7 & 5 \end{bmatrix}$$

If A is a square matrix: 
$$[A] = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

A<sup>T</sup> is the transpose of A 
$$[A]^T = \begin{bmatrix} a_{11} & a_{21} & a_{31} & a_{41} \\ a_{12} & a_{22} & a_{32} & a_{42} \\ a_{13} & a_{23} & a_{33} & a_{43} \\ a_{14} & a_{24} & a_{34} & a_{44} \end{bmatrix}$$



$$\operatorname{tr}\left[A\right] = \sum_{i=1}^{n} a_{ii}$$

tr [A] is the trace of matrix [A]

Ex., A = 
$$\begin{bmatrix} 2 & 3 & 4 \\ 5 & 6 & 7 \\ 8 & 9 & 10 \end{bmatrix}$$

$$tra[A] = 2 + 6 + 10 = 18$$

For a 2 x 2 determinant 
$$D = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

Ex., 
$$D = \begin{vmatrix} 3 & 2 \\ -1 & 2 \end{vmatrix} = 3(2) - 2(-1) = 8$$
For a 3 x 3 determinant 
$$D = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$
 minor  

$$D = a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$
Ex.,  $D = \begin{vmatrix} 0.3 & 0.52 & 1 \\ 0.5 & 1 & 1.9 \\ 0.1 & 0.3 & 0.5 \end{vmatrix}$   
 $D = 0.3 \times \begin{vmatrix} 1 & 1.9 \\ 0.3 & 0.5 \end{vmatrix} - 0.52 \times \begin{vmatrix} 0.5 & 1.9 \\ 0.1 & 0.5 \end{vmatrix} + 1 \times \begin{vmatrix} 0.5 & 1 \\ 0.1 & 0.3 \end{vmatrix}$   
 $D = 0.3 \times (1 \times 0.5 - 0.3 \times 1.9) - 0.52 \times 0.06 + 1 \times 0.05 = -0.0022$ 

#### "Augmentation"

$$\begin{bmatrix} A \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \longrightarrow \begin{bmatrix} A \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & | & 1 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & | & 0 & 1 & 0 \\ a_{31} & a_{32} & a_{33} & | & 0 & 0 & 1 \end{bmatrix}$$

Such an expression has utility when we must perform a set of identical operations on two matrices. Thus, we can perform the operations on the single augmented matrix rather than on the two individual matrices.

 $[A]{X} = {B}$ 

$$[A] = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$
$$\{X\}^T = \lfloor X_1 \quad X_2 \quad \cdots \quad X_n \rfloor$$
$$\{B\}^T = \lfloor b_1 \quad b_2 \quad \cdots \quad b_n \rfloor$$



No division in Matrices

$$[A]{X} = {B}$$

$$[A]^{-1}[A]{X} = [A]^{-1}{B} \qquad [A]^{-1}[A] = [I]$$

$$\{X\} = [A]^{-1}\{B\}$$

# **Solving Linear Algebraic Equations**

> Solving small number of equations:

 $\checkmark$  The Graphical Method.

✓ Cramer's Rule.

 $\checkmark$  The Elimination of Unknowns.

Gauss Elimination

- Gauss-Jordan
- LU Decomposition
- Gauss Seidel

# **Solving Linear Algebraic Equations**

> Direct Methods:

✓ Cramer's Rule.

 $\checkmark$  Gauss Elimination.

✓ Gauss Jordan.

✓ Banded Matrix.

✓ Skyline

Iterative Methods

✓ Jacobi Iteration.

✓ Gauss-Seidel

#### Suitable for small number of equations ( $\leq 3$ )













Is there cases where there will be no solution?



Is there cases where there will be no solution?



#### Is there cases where there will be no solution?







This rule states that each unknown in a system of linear algebraic equations may be expressed as a fraction of two determinants with <u>denominator D</u> and with the <u>numerator obtained from D</u> by <u>replacing</u> the <u>column of</u> <u>coefficients of the unknown</u> in question by the constants  $\underline{b_1}, \underline{b_2}, \ldots, \underline{b_n}$ . For example,  $x_1$  would be computed as:

$$x_{1} = \frac{\begin{vmatrix} b_{1} & a_{12} & a_{13} \\ b_{2} & a_{22} & a_{23} \\ b_{3} & a_{32} & a_{33} \end{vmatrix}}{D}$$



Ex., 
$$0.3x_1 + 0.52x_2 + x_3 = -0.01$$
  
 $0.5x_1 + x_2 + 1.9x_3 = 0.67$   
 $0.1x_1 + 0.3x_2 + 0.5x_3 = -0.44$ 

$$D = \begin{vmatrix} 0.3 & 0.52 & 1 \\ 0.5 & 1 & 1.9 \\ 0.1 & 0.3 & 0.5 \end{vmatrix} = 0.3(-0.07) - 0.52(0.06) + 1(0.05) = -0.0022$$



Ex., 
$$0.3x_1 + 0.52x_2 + x_3 = -0.01$$
  
 $0.5x_1 + x_2 + 1.9x_3 = 0.67$   
 $0.1x_1 + 0.3x_2 + 0.5x_3 = -0.44$   

$$\begin{vmatrix} -0.01 & 0.52 & 1 \\ 0.67 & 1 & 1.9 \\ -0.44 & 0.3 & 0.5 \end{vmatrix} = \frac{0.03278}{-0.0022} = -14.9$$



Ex., 
$$0.3x_1 + 0.52x_2 + x_3 = -0.01$$
  
 $0.5x_1 + x_2 + 1.9x_3 = 0.67$   
 $0.1x_1 + 0.3x_2 + 0.5x_3 = -0.44$   

$$\begin{vmatrix} 0.3 & -0.01 & 1 \\ 0.5 & 0.67 & 1.9 \\ 0.1 & -0.44 & 0.5 \end{vmatrix} = \frac{0.0649}{-0.0022} = -29.5$$



Ex., 
$$0.3x_1 + 0.52x_2 + x_3 = -0.01$$
  
 $0.5x_1 + x_2 + 1.9x_3 = 0.67$   
 $0.1x_1 + 0.3x_2 + 0.5x_3 = -0.44$   

$$\begin{vmatrix} 0.3 & 0.52 & -0.01 \\ 0.5 & 1 & 0.67 \\ -0.44 \end{vmatrix} = \frac{-0.04356}{-0.0022} = 19.8$$

# The Elimination of Unknowns

- The basic strategy is to multiply the equations by constants so that one of the unknowns will be eliminated when the two equations are combined.
- The result is a single equation that can be solved for the remaining unknown.
- This value can then be substituted into either of the original equations to compute the other variable.

## The Elimination of Unknowns



#### The Elimination of Unknowns

Ex., 
$$3x_1 + 2x_2 = 18$$
  
 $-x_1 + 2x_2 = 2$ 

$$x_1 = \frac{a_{22}b_1 - a_{12}b_2}{a_{11}a_{22} - a_{12}a_{21}} = \frac{2(18) - 2(2)}{3(2) - 2(-1)} = 4$$

$$x_2 = \frac{a_{11}b_2 - a_{21}b_1}{a_{11}a_{22} - a_{12}a_{21}} = \frac{3(2) - (-1)18}{3(2) - 2(-1)} = 3$$



The procedure consisted of two steps:

- 1. The equations were manipulated to eliminate one of the unknowns from the equations. The result of this elimination step was that we had one equation with one unknown.
- 2. Consequently, this equation could be solved directly and the result back-substituted into one of the original equations to solve for the remaining unknown.



Ex.,





$$\begin{bmatrix} 3 & -0.1 & -0.2 & 7.85 \\ 0 & 7.00333 & -0.29333 & -19.5617 \\ \hline 0 & 0 & 10.0120 & 70.0843 \end{bmatrix}$$

$$x_3 = \frac{70.0843}{10.0120} = 7.0000$$

$$\begin{bmatrix} 3 & -0.1 & -0.2 & 7.85 \\ \hline 0 & 7.00333 & -0.29333 & -19.5617 \\ \hline 0 & 0 & 10.0120 & 70.0843 \end{bmatrix}$$

 $7.00333x_2 - 0.293333(7.0000) = -19.5617$ 

$$x_2 = \frac{-19.5617 + 0.293333(7.0000)}{7.00333} = -2.50000$$

$$\begin{bmatrix} 3 & -0.1 & -0.2 & 7.85 \\ 0 & 7.00333 & -0.29333 & -19.5617 \\ 0 & 0 & 10.0120 & 70.0843 \end{bmatrix}$$

$$3x_1 - 0.1(-2.50000) - 0.2(7.0000) = 7.85$$

$$x_1 = \frac{7.85 + 0.1(-2.50000) + 0.2(7.0000)}{3} = 3.00000$$

Dividing by zero (or close to zero)

Solution: "Partial pivoting" switch rows and use the largest value as a pivot Pivot=0 $2x_2 + 3x_3 = 8$  $4x_1 + 6x_2 + 7x_3 = -3$  $2x_1 + x_2 + 6x_3 = 5$ 

**Round-off errors** 

Important for more than 100 equations

You should always substitute your answers back into the original equations to check whether a substantial error has occurred.

Solution: scaling & use more significant fraction figures







► Use more significant fraction figures

$$\begin{bmatrix} 2 & 100000 & 100000 \\ 1 & 1 & 2 \end{bmatrix} \Longrightarrow \begin{bmatrix} 2 & 100000 & 100000 \\ 0 & -499999 & -49998 \end{bmatrix}$$
$$\mathbf{x}_{2} = \frac{-499988}{-499999} = 0.999988$$

 $2x_1 + 100,000x0.99998 = 100,000 \implies x_1 = 1$ 

Use scaling that maximum coefficient in each row is 1



- 3. Singular systems (D = 0)
- 4. Ill conditioned systems
  - Ill-conditioning is that a wide range of answers can approximately satisfy the equations.
  - Because round-off errors can induce small changes in the coefficients, these artificial changes can lead to large solution errors for ill-conditioned systems.
  - ▶  $D \approx 0$  (scaling numbers in the matrix to be less than one)
  - Solution: use more significant figures
## **Drawbacks of Gauss Elimination**

Ex., 
$$x_1 + 2x_2 = 10$$
  
 $1.1x_1 + 2x_2 = 10.4$   

$$\begin{bmatrix} 1 & 2 & | & 10 \\ 1.1 & 2 & | & 10.4 \end{bmatrix} \Longrightarrow \begin{bmatrix} 1 & 2 & | & 10 \\ 0 & -0.2 & | & -0.6 \end{bmatrix}$$
 $x_2 = \frac{-0.6}{-0.2} = 3$   
 $x_1 + 2x_3 = 10 \implies x_1 = 4$ 

## **Drawbacks of Gauss Elimination**

Replace 1.1 by 1.05

$$\begin{bmatrix} 1 & 2 & 10 \\ 1.05 & 2 & 10.4 \end{bmatrix} \Longrightarrow \begin{bmatrix} 1 & 2 & 10 \\ 0 & -0.1 & -0.1 \end{bmatrix}$$
$$\mathbf{x}_2 = \frac{-0.1}{-0.1} = 1$$
$$\mathbf{x}_1 + 2x\mathbf{1} = 1\mathbf{0} \implies \mathbf{x}_1 = \mathbf{8}$$

## **Drawbacks of Gauss Elimination**



## **Gauss Elimination**

