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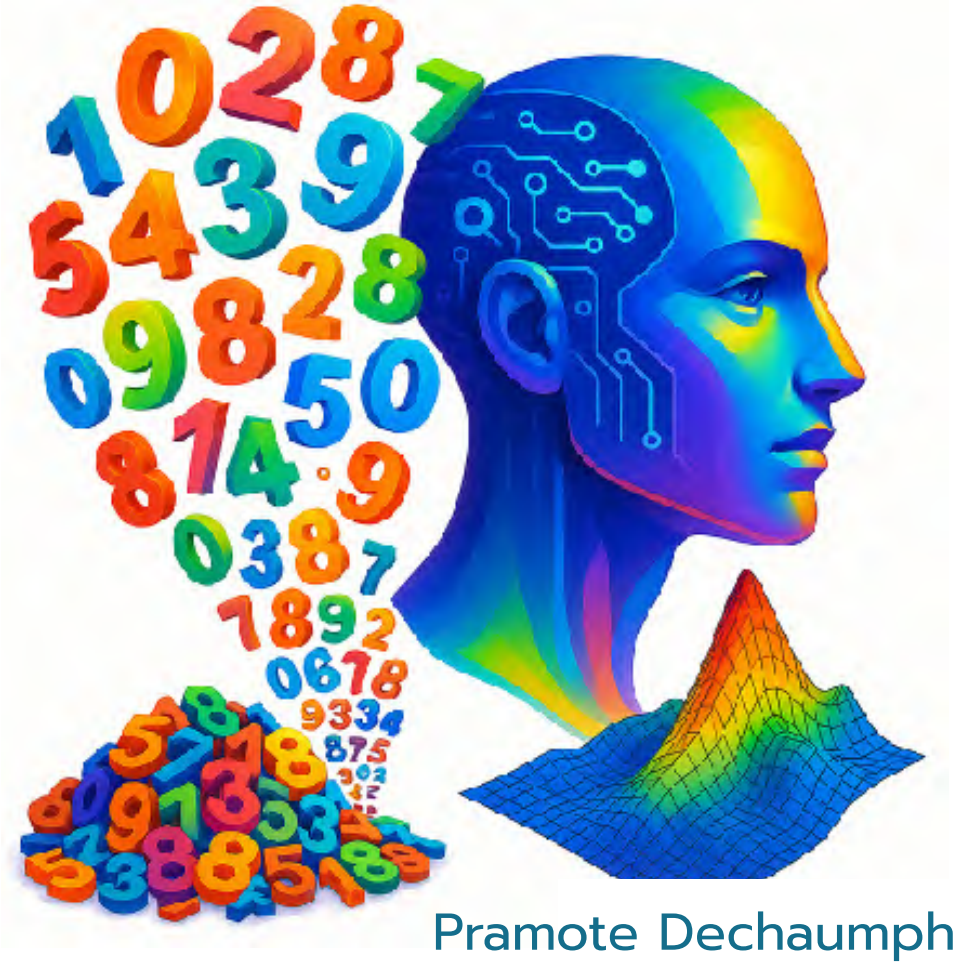
NUMERICAL METHODS with AI

From Fundamentals to Finite Difference, Finite Element, and Finite Volume Methods



Pramote Dechaumphai

Numerical Methods with AI

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Preface

Artificial Intelligence (AI) now offers an efficient way to solve problems in numerical methods taught at the university level. Numerical methods form the foundation of advanced computational techniques used in industrial and research software. This book, *Numerical Methods with AI*, presents concise explanations of the key concepts in each method to help readers gain a clear overall understanding. It then demonstrates computational procedures and solutions generated by AI, allowing learners to grasp the methods quickly and verify the accuracy of AI-generated results.

This book is written in a concise format with a limited number of pages to make it affordable and accessible. Users of advanced computational software can easily study from it to gain a better understanding of the underlying methods embedded in commercial software, which often do not explain their theoretical background in detail.

The author would like to express sincere appreciation to Chulalongkorn University Press for supporting the publication and distribution of this book, which aims to promote knowledge and understanding of the use of AI in numerical methods. It is the author's hope that this book will inspire readers to apply AI to more advanced levels of numerical analysis.

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*** Precautions in Using AI ***

Numerical methods require knowledge and understanding of mathematics and computation. This book is designed to develop these skills through step-by-step explanations that promote quick understanding. Each chapter includes examples that demonstrate problem-solving procedures, allowing readers to verify the results generated by AI. Therefore, to achieve effective learning. Readers should always keep in mind that:

- Problems should be solved manually before using AI to verify the answers.
- Questions should be asked to AI to clarify and deepen the understanding of the results.
- Problems should not be given to AI solely to obtain answers. Understanding the methods is the essence of learning numerical methods.
- AI-generated answers should not always be trusted, as AI can be wrong. Always verify the answers.
- Study computer programs generated by AI to enhance advanced programming skills. Since specialized software is often unavailable or highly expensive, developing programs independently fosters both a sense of achievement and meaningful opportunities for continued learning.

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Chapter 1

Linear Algebraic Equations

1.1 Introduction

The numerical methods commonly employed to solve problems in science and engineering include the Finite Difference Method (FDM), the Finite Element Method (FEM), and the Finite Volume Method (FVM). These techniques convert differential equations into systems of algebraic equations that involve only basic arithmetic operations such as addition, subtraction, multiplication, and division. Therefore, they can be efficiently solved using computer programs. In practical applications, such algebraic systems may range from hundreds to millions of equations. These systems can be generally represented in the following standard form:

$$\underset{(n\times n)}{[A]}\ \underset{(n\times 1)}{\{X\}} \;=\; \underset{(n\times 1)}{\{B\}}$$

where n is the number of equations, $[A]$ is an $(n\times n)$ square matrix consisting of known numerical coefficients, $\{X\}$ is a column vector containing n unknown variables, and $\{B\}$ is also a column vector containing n known numerical values.

In this chapter, we will study methods for solving systems of algebraic equations in the above form. We will first understand the principles behind each

method before using AI to solve the same problem. Doing so will help us grasp the overall computational process and enable us to verify the correctness of AI-generated results. The solution of the system of equations $[A]\{X\} = \{B\}$ can be approached in two main ways: (1) Direct methods, and (2) Iterative methods. Since these methods can be applied to systems ranging from a few to many equations, we will use an example consisting of three equations, which allows us to clearly understand each method in detail, as follows:

$$\begin{bmatrix} 4 & -2 & -1 \\ -3 & 6 & -2 \\ -2 & -1 & 8 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 7 \\ 1 \\ 0 \end{Bmatrix}$$

The solution of these three equations are: $x_1 = 3$, $x_2 = 2$ and $x_3 = 1$.

1.2 Cramer's Rule

Cramer' s rule is a method used for solving systems of equations that contain only a small number of unknowns. The fundamental principle of this method is that each unknown variable can be determined directly from the determinants of the corresponding matrices as,

$$x_i = \frac{\det[A]_i}{\det[A]}$$

where $\det[A]$ is the determinant of matrix $[A]$, and $\det[A]_i$ is the determinant of the matrix obtained by replacing the i^{th} column of $[A]$ with the vector $\{B\}$. By using Cramer's rule with the above equations, we can ask ChatGPT to show the step- by- step calculation to obtain the solution, as illustrated in the following example.

Example Use the Cramer's rule to solve the following set of algebraic equations,

$$\begin{bmatrix} 4 & -2 & -1 \\ -3 & 6 & -2 \\ -2 & -1 & 8 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 7 \\ 1 \\ 0 \end{Bmatrix}$$

We can use ChatGPT by simply entering the following text after the prompt.

Given [A] = [4 -2 -1; -3 6 -2; -2 -1 8], {B} = [7; 1; 0] and {X} = [x1; x2; x3] Use Cramer's Rule to solve for {X}. Show the step-by-step derivation in detail.

ChatGPT will display the computational steps to obtain the solutions as follows.

We will use *Cramer's Rule* to solve $AX = B$,

Given: $A=\begin{bmatrix} 4 & -2 & -1 \\ -3 & 6 & -2 \\ -2 & -1 & 8 \end{bmatrix}, \quad B=\begin{bmatrix} 7 \\ 1 \\ 0 \end{bmatrix}, \quad X=\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$

1) Compute det A

Expand along row 1 (cofactors $C_{ij}=(-1)^{i+j}M_{ij}$):

- $M_{11} = \begin{vmatrix} 6 & -2 \\ -1 & 8 \end{vmatrix} = 48-2 = 46 \Rightarrow C_{11} = +46$
- $M_{12} = \begin{vmatrix} -3 & -2 \\ -2 & 8 \end{vmatrix} = -24-4 = -28 \Rightarrow C_{12} = -(-28) = +28$
- $M_{13} = \begin{vmatrix} -3 & 6 \\ -2 & -1 \end{vmatrix} = 3-(-12) = 15 \Rightarrow C_{13} = +15$

$$\det A = 4(46)+(-2)(28)+(-1)(15) = 184-56-15 = 113.$$

2) Matrix A_1 (replace col 1 by B) and det A_1

$$A_1=\begin{bmatrix} 7 & -2 & -1 \\ 1 & 6 & -2 \\ 0 & -1 & 8 \end{bmatrix}.$$

Expand down column 1 (has a zero):

- $C_{11} = +\begin{vmatrix} 6 & -2 \\ -1 & 8 \end{vmatrix} = 46 \Rightarrow 7 \cdot 46 = 322$
- $C_{21} = -\begin{vmatrix} -2 & -1 \\ -1 & 8 \end{vmatrix} = -(-16-1) = +17 \Rightarrow 1 \cdot 17 = 17$

$$\det A_1 = 322+17 = 339.$$

3) Matrix A_2 (replace col 2 by B) and det A_2

$$A_2=\begin{bmatrix} 4 & 7 & -1 \\ -3 & 1 & -2 \\ -2 & 0 & 8 \end{bmatrix}.$$

Expand down column 2 (has a zero):

- $C_{12} = -\begin{vmatrix} -3 & -2 \\ -2 & 8 \end{vmatrix} = -(-24-4) = +28 \Rightarrow 7 \cdot 28 = 196$

- $C_{22} = +\begin{vmatrix} 4 & -1 \\ -2 & 8 \end{vmatrix} = 32-2 = 30 \Rightarrow 1 \cdot 30 = 30$

$$\det A_2 = 196+30 = 226.$$

4) Matrix A_3 (replace col 3 by B) and $\det A_3$

$$A_3 = \begin{bmatrix} 4 & -2 & 7 \\ -3 & 6 & 1 \\ -2 & -1 & 0 \end{bmatrix}.$$

Expand down column 3 (has a zero):

- $C_{13} = +\begin{vmatrix} -3 & 6 \\ -2 & -1 \end{vmatrix} = 3-(-12) = 15 \Rightarrow 7 \cdot 15 = 105$
- $C_{23} = -\begin{vmatrix} 4 & -2 \\ -2 & -1 \end{vmatrix} = -(-4-4) = +8 \Rightarrow 1 \cdot 8 = 8$

$$\det A_3 = 105+8 = 113.$$

5) Solve for x_1, x_2, x_3

$$x_1 = \frac{\det A_1}{\det A} = \frac{339}{113} = 3, \quad x_2 = \frac{\det A_2}{\det A} = \frac{226}{113} = 2, \quad x_3 = \frac{\det A_3}{\det A} = \frac{113}{113} = 1.$$

$$X = \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}$$

Although the above example shows that using Cramer's rule is indeed a simple way to find solutions, this method is not commonly used in practice. The main reason is that it requires significantly more computation time compared to other methods that will be introduced later. The number of arithmetic operations (addition, subtraction, multiplication, and division) required by Cramer's rule is approximately $(n-1)\cdot(n+1)!$ where n is the number of equations. For instance, if the system contains 100 equations, the total number of arithmetic operations would be around 10^{157}, which is an astronomically large number, making the method impractical for real applications. In the next section, we will study the Gauss elimination method, which drastically reduces the number of arithmetic operations to approximately $(2n^3/3)+(3n^2/2)-(7n/6)$. That means for a system of 100 equations, only about 700,000 operations are needed, a much more efficient approach in practice.

1.3 Gauss Elimination Method

The Gauss elimination method is one of the most widely used techniques for solving systems of linear equations. It is a standard approach employed in large-scale computer programs designed to solve engineering and scientific problems. In general, the Gauss elimination method can be divided into two main stages:

(a) *Forward elimination*: Suppose we have a system consisting of three linear equations as follows,

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

Forward elimination is the process of transforming the original system of equations into a form in which the square matrix on the left-hand side becomes an upper triangular matrix. That is, a matrix whose elements below the main diagonal are all zeros as,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a''_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b'_2 \\ b''_3 \end{Bmatrix}$$

The prime symbol ($'$) on a coefficient indicates that the coefficient has been updated, that is, its value has changed from the original one.

(b) *Back Substitution*: Once the system of equations has been transformed into the new form, it becomes straightforward to calculate the unknown variables. The computation begins with the last equation and proceeds upward, determining each variable of x_i one by one as follows,

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

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

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

Example Use the Gauss elimination method to solve the following set of equations,

$$\begin{bmatrix} 4 & -2 & -1 \\ -3 & 6 & -2 \\ -2 & -1 & 8 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 7 \\ 1 \\ 0 \end{Bmatrix}$$

We can use ChatGPT by simply entering the following text after the prompt.

Given [A] = [4 -2 -1; -3 6 -2; -2 -1 8], {B} = [7; 1; 0] and {X} = [x1; x2; x3] Use Gauss Elimination Method to solve for {X}. Show the step- by- step derivation in detail.

ChatGPT will display the computational steps to obtain the solutions as follows.

Let's solve $Ax = B$ by *Gaussian Elimination Method*.

$$A = \begin{bmatrix} 4 & -2 & -1 \\ -3 & 6 & -2 \\ -2 & -1 & 8 \end{bmatrix}, \quad B = \begin{bmatrix} 7 \\ 1 \\ 0 \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

1) Set up the augmented matrix and do forward elimination:

$$\left[\begin{array}{ccc|c} 4 & -2 & -1 & 7 \\ -3 & 6 & -2 & 1 \\ -2 & -1 & 8 & 0 \end{array}\right]$$

Use the pivot $a_{11} = 4$ to eliminate below it.

$R_2 \leftarrow R_2 + \frac{3}{4} R_1$:

$R_2 = \left[-3+3,\ 6-\frac{3}{2},\ -2-\frac{3}{4} \mid 1+\frac{21}{4}\right] = \left[0,\ \frac{9}{2},\ -\frac{11}{4} \mid \frac{25}{4}\right]$

$R_3 \leftarrow R_3 + \frac{1}{2} R_1$:

$R_3 = \left[-2+2,\ -1-1,\ 8-\frac{1}{2} \mid 0+\frac{7}{2}\right] = \left[0,\ -2,\ \frac{15}{2} \mid \frac{7}{2}\right]$

Now:
$$\left[\begin{array}{ccc|c} 4 & -2 & -1 & 7 \\ 0 & \frac{9}{2} & -\frac{11}{4} & \frac{25}{4} \\ 0 & -2 & \frac{15}{2} & \frac{7}{2} \end{array}\right]$$

Use the pivot $a_{22} = \frac{9}{2}$ to eliminate a_{32}.

Factor $= \dfrac{-2}{9/2} = -\dfrac{4}{9}$ and $R3 \leftarrow R_3 - (-\frac{4}{9})R_2 = R_3 + \frac{4}{9} R_2$:

- New $a_{32} = -2 + \frac{4}{9} \cdot \frac{9}{2} = 0$ (as intended)
- New $a_{33} = \frac{15}{2} + \frac{4}{9} \cdot (-\frac{11}{4}) = \frac{15}{2} - \frac{11}{9} = \frac{113}{18}$
- New RHS $= \frac{7}{2} + \frac{4}{9} \cdot \frac{25}{4} = \frac{7}{2} + \frac{25}{9} = \frac{113}{18}$

So:
$$\left[\begin{array}{ccc|c} 4 & -2 & -1 & 7 \\ 0 & \frac{9}{2} & -\frac{11}{4} & \frac{25}{4} \\ 0 & 0 & \frac{113}{18} & \frac{113}{18} \end{array}\right]$$

2) Back substitution

From row 3:

$$\frac{113}{18}x_3 = \frac{113}{18} \Rightarrow x_3 = 1.$$

From row 2:

$$\frac{9}{2}x_2 - \frac{11}{4}x_3 = \frac{25}{4} \Rightarrow \frac{9}{2}x_2 - \frac{11}{4} = \frac{25}{4} \Rightarrow \frac{9}{2}x_2 = \frac{36}{4} = 9 \Rightarrow x_2 = 2.$$

From row 1:

$$4x_1 - 2x_2 - x_3 = 7 \Rightarrow 4x_1 - 4 - 1 = 7 \Rightarrow 4x_1 = 12 \Rightarrow x_1 = 3. \qquad x = \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}$$

1.4 Gauss-Jordan Method

The Gauss-Jordan method is an extension of the Gauss elimination method. For example, suppose we have a system consisting of three linear equations as before,

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

The process begins with *forward elimination*, similar to that used in the Gauss elimination method. The original system of equations is then transformed into a form in which the square matrix on the left-hand side contains zeros throughout both the lower-left and upper-right portions, while all elements along the main diagonal are equal to one as,

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1^* \\ b_2^* \\ b_3^* \end{Bmatrix}$$

This transformation immediately yields the following result,

$$\begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1^* \\ b_2^* \\ b_3^* \end{Bmatrix}$$

Example Use the Gauss-Jordan method to solve the following set of equations,

$$\begin{bmatrix} 4 & -2 & -1 \\ -3 & 6 & -2 \\ -2 & -1 & 8 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 7 \\ 1 \\ 0 \end{Bmatrix}$$

We can use ChatGPT by simply entering the following text after the prompt.

Given [A] = [4 -2 -1; -3 6 -2; -2 -1 8], {B} = [7; 1; 0] and {X} = [x1; x2; x3] Use Gauss-Jordan Elimination Method to solve for {X}. Show the step-by-step derivation in detail.

ChatGPT will display the computational steps to obtain the solutions as follows.

We are solving the linear system: $AX = B$

where: $$A = \begin{bmatrix} 4 & -2 & -1 \\ -3 & 6 & -2 \\ -2 & -1 & 8 \end{bmatrix}, \quad B = \begin{bmatrix} 7 \\ 1 \\ 0 \end{bmatrix}, \quad X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Using the *Gauss-Jordan Elimination Method*, we augment matrix A with column B and reduce it.

Step 1: Write the augmented matrix $[A \mid B]$

$$\left[\begin{array}{ccc|c} 4 & -2 & -1 & 7 \\ -3 & 6 & -2 & 1 \\ -2 & -1 & 8 & 0 \end{array}\right]$$

Step 2: Make the pivot of Row 1 a 1 (means taking the first non-zero number (called the pivot) in Row 1, and scaling the entire row so that this number becomes 1) Divide Row 1 by 4:

- $R_1 \leftarrow \frac{1}{4} R_1$

$$\left[\begin{array}{ccc|c} 1 & -0.5 & -0.25 & 1.75 \\ -3 & 6 & -2 & 1 \\ -2 & -1 & 8 & 0 \end{array}\right]$$

Step 3: Eliminate elements below pivot in column 1

- $R_2 \leftarrow R_2 + 3 \cdot R_1$
- $R_3 \leftarrow R_3 + 2 \cdot R_1$

$$\left[\begin{array}{ccc|c} 1 & -0.5 & -0.25 & 1.75 \\ 0 & 4.5 & -2.75 & 6.25 \\ 0 & -2 & 7.5 & 3.5 \end{array}\right]$$

Step 4: Make the pivot of Row 2 a 1 (means taking the first non-zero number (pivot) in Row 2, and scaling (dividing) the entire row so that this number becomes 1)
Divide Row 2 by 4.5:

- $R_2 \leftarrow 14.5R2$

$$\left[\begin{array}{ccc|c} 1 & -0.5 & -0.25 & 1.75 \\ 0 & 1 & -0.6111 & 1.3889 \\ 0 & -2 & 7.5 & 3.5 \end{array}\right]$$

Step 5: Eliminate above and below pivot in column 2

- $R_1 \leftarrow R1 + 0.5 \cdot R_2$
- $R_3 \leftarrow R_3 + 2 \cdot R_2$

$$\left[\begin{array}{ccc|c} 1 & 0 & -0.5556 & 2.4444 \\ 0 & 1 & -0.6111 & 1.3889 \\ 0 & 0 & 6.2778 & 6.2778 \end{array}\right]$$

Step 6: Make pivot of Row 3 a 1 (means taking the first non-zero number (called the pivot) in Row 3 and dividing entire row by that number to make it equal to 1)

- $R_3 \leftarrow 16.2778R_3$

$$\left[\begin{array}{ccc|c} 1 & 0 & -0.5556 & 2.4444 \\ 0 & 1 & -0.6111 & 1.3889 \\ 0 & 0 & 1 & 1 \end{array}\right]$$

Step 7: Eliminate above pivot in column 3

- $R_1 \leftarrow R_1 + 0.5556 \cdot R_3$
- $R_2 \leftarrow R_2 + 0.6111 \cdot R_3$

$$\left[\begin{array}{ccc|c} 1 & 0 & 0 & 3 \\ 0 & 1 & 0 & 2 \\ 0 & 0 & 1 & 1 \end{array}\right]$$

Final Solution:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}$$

Answer: $x_1 = 3, \quad x_2 = 2, \quad x_3 = 1$

1.5 Matrix Inversion

The matrix inverse of a given matrix can be conveniently obtained using the Gauss-Jordan method. Suppose we are given a (3×3) matrix as follows,

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

and we wish to find its inverse matrix $[A]^{-1}$. We begin with the fundamental relationship,

$$\underset{(3\times3)}{[A]}\,\underset{(3\times3)}{[A]^{-1}} = \underset{(3\times3)}{[I]}$$

where $[I]$ denotes the identity matrix. If we let the inverse matrix $[A]^{-1}$ consisting of three column matrices as,

$$\underset{(3\times3)}{[A]^{-1}} = \left[\underset{(3\times1)}{\{X\}_1} \quad \underset{(3\times1)}{\{X\}_2} \quad \underset{(3\times1)}{\{X\}_3}\right]$$

and substitute back into the above equation, we obtain,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \left[\begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix}_1 \quad \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix}_2 \quad \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix}_3 \right] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

This implies that we must solve the system of equations three times. That is, as if there are three different right-hand side vectors as,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 0 \\ 0 \end{Bmatrix}, \begin{Bmatrix} 0 \\ 1 \\ 0 \end{Bmatrix}, \begin{Bmatrix} 0 \\ 0 \\ 1 \end{Bmatrix}$$

Since this system consists of different right-hand side vectors but shares the same square matrix on the left-hand side, we can apply the Gauss-Jordan method to perform the forward elimination simultaneously for all three vectors, as illustrated in the following example.

Example Determine the inverse matrix $[A]^{-1}$ from the matrix,

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

We can use ChatGPT by simply entering the following text after the prompt.

Given [A] = [4 -2 -1; -3 6 -2; -2 -1 8]. Find the inverse [A]. Show the step-by-step derivation in detail.

ChatGPT will display the computational steps to obtain the solutions as follows.

To find the *inverse of matrix*:

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

We will use the *Gauss-Jordan elimination* method by transforming $[A|\,I]$ into $[I|A^{-1}]$.

Step 1: Form the augmented matrix $[A|\,I]$

$$\left[\begin{array}{ccc|ccc} 4 & -2 & -1 & 1 & 0 & 0 \\ -3 & 6 & -2 & 0 & 1 & 0 \\ -2 & -1 & 8 & 0 & 0 & 1 \end{array}\right]$$

Step 2: Make the pivot of Row 1 equal to 1
Divide Row 1 by 4:

$$R_1 \leftarrow \frac{1}{4}R_1 \quad \Rightarrow \quad \left[\begin{array}{ccc|ccc} 1 & -\frac{1}{2} & -\frac{1}{4} & \frac{1}{4} & 0 & 0 \\ -3 & 6 & -2 & 0 & 1 & 0 \\ -2 & -1 & 8 & 0 & 0 & 1 \end{array}\right]$$

Step 3: Eliminate entries below the pivot (column 1)
$R_2 \leftarrow R_2 + 3 \cdot R_1$ and $R_3 \leftarrow R_3 + 2 \cdot R_1$

Updated matrix:

$$\left[\begin{array}{ccc|ccc} 1 & -\frac{1}{2} & -\frac{1}{4} & \frac{1}{4} & 0 & 0 \\ 0 & \frac{9}{2} & -\frac{11}{4} & \frac{3}{4} & 1 & 0 \\ 0 & -2 & \frac{15}{2} & \frac{1}{2} & 0 & 1 \end{array}\right]$$

Step 4: Make pivot of Row 2 = 1
Divide Row 2 by $\frac{9}{2}$ $\Rightarrow$ $R_2 \leftarrow \frac{2}{9}R_2$

So:

$$\left[\begin{array}{ccc|ccc} 1 & -\frac{1}{2} & -\frac{1}{4} & \frac{1}{4} & 0 & 0 \\ 0 & 1 & -\frac{11}{18} & \frac{1}{6} & \frac{2}{9} & 0 \\ 0 & -2 & \frac{15}{2} & \frac{1}{2} & 0 & 1 \end{array}\right]$$

Step 5: Eliminate above and below pivot in column 2

Row 1: $R_1 \leftarrow R_1 + \frac{1}{2}R_2$ and Row 3: $R_3 \leftarrow R_3 + 2R_2$

Updated matrix:
$$\left[\begin{array}{ccc|ccc} 1 & 0 & -\frac{5}{9} & \frac{1}{3} & \frac{1}{9} & 0 \\ 0 & 1 & -\frac{11}{18} & \frac{1}{6} & \frac{2}{9} & 0 \\ 0 & 0 & \frac{91}{18} & \frac{5}{6} & \frac{4}{9} & 1 \end{array}\right]$$

Step 6: Make pivot of Row 3 = 1

$$R_3 \leftarrow \frac{18}{91}R_3$$

New Row 3:
$$\left[\begin{array}{ccc|ccc} 0 & 0 & 1 & \frac{15}{91} & \frac{8}{91} & \frac{18}{91} \end{array}\right]$$

Step 7: Eliminate above (column 3)

Row 1: $R_1 \leftarrow R_1 + \frac{5}{9}R_3$ and Row 2: $R_2 \leftarrow R_2 + \frac{11}{18}R_3$

Final augmented matrix:
$$\left[\begin{array}{ccc|ccc} 1 & 0 & 0 & \frac{116}{273} & \frac{131}{819} & \frac{10}{91} \\ 0 & 1 & 0 & \frac{64}{273} & \frac{10}{91} & \frac{18}{91} \\ 0 & 0 & 1 & \frac{15}{91} & \frac{8}{91} & \frac{18}{91} \end{array}\right]$$

Final Answer:

The inverse of A is:
$$A^{-1} = \begin{bmatrix} \frac{116}{273} & \frac{131}{819} & \frac{10}{91} \\ \frac{64}{273} & \frac{10}{91} & \frac{18}{91} \\ \frac{15}{91} & \frac{8}{91} & \frac{18}{91} \end{bmatrix}$$

1.6 LU Decomposition Method

The LU decomposition method is another widely used approach for solving systems of equations in practical applications. The basic concept of this method is

straightforward and can be understood by starting from the system of equations to be solved,

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

The first step is to decompose the matrix $[A]$ into the product of two matrices, $[L]$ and $[U]$, as,

$$[A] = [L][U]$$

For example, if the system consists of only three equations, the detailed structure of these matrices is as follows,

$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}}_{[A]} = \underbrace{\begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} \end{bmatrix}}_{[L]} \underbrace{\begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix}}_{[U]}$$

That is, the matrix $[L]$ is a *lower triangular matrix* whose elements above the main diagonal are all zeros, while the matrix $[U]$ is an *upper triangular matrix* whose elements below the main diagonal are all zeros. Substituting the matrix $[A]=[L][U]$ back into the original equation gives,

$$[L]\underbrace{[U]\{X\}}_{\{Y\}} = \{B\}$$

Therefore, we can solve the system of equations,

$$[L]\{Y\} = \{B\}$$

first, by performing forward substitution to determine the vector $\{Y\}$. After that, we solve the system of equations,

$$[U]\{X\} = \{Y\}$$

by performing backward substitution to find the result of $\{X\}$.

From this explanation, we can see that solving the system of equations $[A]\{X\}=\{B\}$ using the LU decomposition method involves three main steps:

(a) Decompose the matrix $[A]$ into the product of two matrices, $[L]$ and $[U]$.

(b) Solve the system $[L]\{Y\}=\{B\}$ by forward substitution to determine the vector $\{Y\}$.

(c) Solve the system $[U]\{X\} = \{Y\}$ by back substitution to obtain the solution vector $\{X\}$.

It should be noted that in the decomposition of matrix $[A]$ into matrices $[L]$ and $[U]$, as shown in the previous equations, the elements along the main diagonal of matrix $[L]$ can take arbitrary values, while those along the main diagonal of matrix $[U]$ are all equal to one. This arrangement of $[L]$ and $[U]$ is referred to as the *Crout decomposition*. Conversely, if the diagonal elements of matrix $[L]$ are all equal to one, while those of matrix $[U]$ take arbitrary values, the resulting form is called the *Doolittle decomposition*. Both forms of decomposition yield the same solution vector $\{X\}$.

Example Use the Crout LU decomposition method to solve the following set of the algebraic equations,

$$\begin{bmatrix} 4 & -2 & -1 \\ -3 & 6 & -2 \\ -2 & -1 & 8 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 7 \\ 1 \\ 0 \end{Bmatrix}$$

We can use ChatGPT by simply entering the following text after the prompt.

Given [A] = [4 -2 -1; -3 6 -2; -2 -1 8], {B} = [7; 1; 0] and {X} = [x1; x2; x3] Use LU Decomposition Method (Crout Method) to solve for {X}. Show the step-by-step derivation in detail.

ChatGPT will display the computational steps to obtain the solutions as follows.

We will use the *Crout's LU Decomposition* (lower-triangular *L* with non-unit diagonal, and unit upper-triangular *U*) so that

$$A = LU, \quad L = \begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} \end{bmatrix}, \qquad U = \begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix}.$$

$$A = \begin{bmatrix} 4 & -2 & -1 \\ -3 & 6 & -2 \\ -2 & -1 & 8 \end{bmatrix}, \qquad B = \begin{bmatrix} 7 \\ 1 \\ 0 \end{bmatrix}.$$

1) Crout factorization *A=LU*

Crout formulas (column by column):

$$\ell_{ij} = a_{ij} - \sum_{k=1}^{j-1} \ell_{ik} u_{kj}, \quad (i \geq j), \qquad u_{ij} = \frac{1}{\ell_{ii}} \left(a_{ij} - \sum_{k=1}^{i-1} \ell_{ik} u_{kj} \right), \quad (i < j).$$

Column j=1:

$$\ell_{11} = a_{11} = 4, \quad \ell_{21} = a_{21} = -3, \quad \ell_{31} = a_{31} = -2.$$

$$u_{12} = \frac{a_{12}}{\ell_{11}} = \frac{-2}{4} = -\tfrac{1}{2}, \qquad u_{13} = \frac{a_{13}}{\ell_{11}} = \frac{-1}{4} = -\tfrac{1}{4}.$$

Column j=2:

$$\ell_{22} = a_{22} - \ell_{21} u_{12} = 6 - (-3)\left(-\tfrac{1}{2}\right) = 6 - \tfrac{3}{2} = \tfrac{9}{2},$$

$$\ell_{32} = a_{32} - \ell_{31} u_{12} = -1 - (-2)\left(-\tfrac{1}{2}\right) = -1 - 1 = -2.$$

$$u_{23} = \frac{a_{23} - \ell_{21} u_{13}}{\ell_{22}} = \frac{-2 - (-3)(-\tfrac{1}{4})}{9/2} = \frac{-2 - \tfrac{3}{4}}{9/2} = \frac{-11/4}{9/2} = -\tfrac{11}{18}.$$

Column j=3:

$$\ell_{33} = a_{33} - \ell_{31} u_{13} - \ell_{32} u_{23} = 8 - (-2)\left(-\tfrac{1}{4}\right) - (-2)\left(-\tfrac{11}{18}\right) = 8 - \tfrac{1}{2} - \tfrac{11}{9} = \tfrac{113}{18}.$$

Thus,

$$L = \begin{bmatrix} 4 & 0 & 0 \\ -3 & \frac{9}{2} & 0 \\ -2 & -2 & \frac{113}{18} \end{bmatrix}, \qquad U = \begin{bmatrix} 1 & -\frac{1}{2} & -\frac{1}{4} \\ 0 & 1 & -\frac{11}{18} \\ 0 & 0 & 1 \end{bmatrix}.$$

2) Forward substitution for $Ly=B$

Let $y = [y_1, y_2, y_3]^T$.

- Row 1: $4y_1 = 7 \Rightarrow y_1 = \frac{7}{4}$.
- Row 2: $-3y_1 + \frac{9}{2} y_2 = 1 \Rightarrow \frac{9}{2} y_2 = 1 + \frac{21}{4} = \frac{25}{4} \Rightarrow y_2 = \frac{25}{18}$.
- Row 3: $-2y_1 - 2y_2 + \frac{113}{18} y_3 = 0 \Rightarrow \frac{113}{18} y_3 = 2y_1 + 2y_2 = \frac{7}{2} + \frac{25}{9} = \frac{113}{18} \Rightarrow y_3 = 1$.

So:
$$y = \begin{bmatrix} \frac{7}{4} \\ \frac{25}{18} \\ 1 \end{bmatrix}.$$

3) Back substitution for $Ux = y$ (unit U)

- Row 3: $x_3 = y_3 = 1$.
- Row 2: $x_2 - \frac{11}{18} x_3 = y_2 \Rightarrow x_2 = \frac{25}{18} + \frac{11}{18} = 2$.
- Row 1: $x_1 - \frac{1}{2} x_2 - \frac{1}{4} x_3 = y_1 \Rightarrow x_1 = \frac{7}{4} + \frac{1}{2} \cdot 2 + \frac{1}{4} = 3$.