Chapter V: Direct Solution of Systems of Linear Equations

The problem of solving systems of linear equations is frequently encountered. These systems are present, for example, in various numerical methods for solving partial differential equations. The latter model the majority of physical phenomena such as heat and mass transfer, fluid mechanics, etc. In this chapter, we will address systems of linear equations where the number of equations is equal to the number of unknowns and where the determinant is non-zero. That is, systems that have a unique solution. A system of linear equations with n equations and n unknowns is then written as:

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots a_{2n}x_n = b_2 \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots. \\ a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots a_{nn}x_n = b_n \end{cases}$$

This system can be written in matrix form:

$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & a_{1n} \\ a_{21} & a_{22} \cdots & a_{2n} \\ & \vdots & \\ a_{n1} & a_{n2} \dots & a_{nn} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}}_{X} = \underbrace{\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}}_{B} \Leftrightarrow AX = B$$

This system can be solved directly by various methods, including Cramer's rule (using determinants) or elimination.

<u>Systems with triangular matrices</u>

Let's start with some definitions. We say that a system UX=Y is a system with an upper triangular matrix if $u_{ij} = 0 \text{ for } \; i > j$:

$$\begin{cases} u_{11}x_1 + u_{12}x_2 + u_{13}x_3 + \cdots + u_{1n}x_n = y_1 \\ \qquad\quad u_{22}x_2 + u_{23}x_3 + \cdots + u_{2n}x_n = y_2 \\ \qquad\qquad\qquad u_{33}x_3 + \cdots + u_{3n}x_n = y_3 \\ \qquad\qquad\qquad\qquad \dots\dots\dots\dots\dots\dots\dots\dots\dots. \\ \qquad\qquad\qquad\qquad\qquad\qquad u_{nn}x_n = y_n \end{cases}$$

The solution of this system is easily calculated by backward substitution. From equation n, we calculate: $x_n = y_n/u_{nn}$

We substitute x_n into equation n-1 to calculate $x_{n-1} = (y_{n-1} - u_{n-1n}x_n)/u_{n-1n-1}$.

For the calculation of x_i, the components $x_n, x_{n-1}, x_{n-2}, \dots., x_{i+1}$ are known, we substitute them into equation i, which gives:

$$x_i = (y_i - \sum_{j=i+1}^{n} u_{ij}x_j)/u_{ii} \quad i=n-1,\ n-2, \dots., 1.$$

The determinant of a triangular matrix (upper or lower) is the product of the diagonal (pivot) elements of that matrix.

$$\det(U) = \prod_{i=1}^{n} u_{ii} = u_{11}u_{22} \dots. u_{nn}$$

Example: Consider the following system of equations:

$$\begin{cases} x - y + z = 1 \\ \qquad\quad 3z = 3 \\ \quad 2y - z = 1 \end{cases}$$

1. Write the system in matrix form.
2. Find the solution of the system.
3. Calculate the determinant of the system's matrix.

Solution

1. Writing the system in matrix form by permuting rows 2 and 3 to obtain an upper triangular system. Let's not forget that the determinant will be multiplied by -1 due to the permutation.

$$A = \begin{bmatrix} 1 & -1 & 1 \\ 0 & 2 & -1 \\ 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 3 \end{bmatrix}$$

2. Backward substitution gives:

$eq.3 : z = \frac{3}{3} = 1,\ \ eq.2 : y = \frac{1+1}{2} = 1\ \ and\ \ x = 1 + 1 - 1 = 1.$

3. $\text{Det(A)} = (-1) * 1 * 2 * 3 = -6.$

<u>5.1 Gaussian Elimination Method</u>

In this chapter, we will start with the Gaussian elimination method, which is similar to the elimination method with a very important modification that greatly facilitates the solution even of large systems (thousands or even millions). This modification transforms a system with a full matrix A into another system with an upper triangular matrix U, such that the two systems AX=B and UX=Y are equivalent, i.e., have the same solution.

Linear algebra shows that certain transformations applied to systems of equations do not change their solutions. In our case, the operations we will apply are the following:

- Multiplication of equation E_i by a non-zero constant α, the new equation obtained $E_{in} = \alpha E_i$ will replace the old E_i.
- Multiplication of equation E_j by a non-zero α and its addition to E_i, $\ E_{in} = E_i + \alpha E_j$, the equation obtained E_{in} will replace E_i.
- Permutation of equations E_i and E_j.

Applying a series of these operations will transform the system AX=B into UX=Y, and then backward substitution will give the solution of the system.

<u>5.1.1 Description of the Gaussian Elimination Method</u>

We will show how to apply the transformations to the system AX=B. For this, the right-hand side B will be considered as the (n+1)th column and will also be affected by the operations. We divide the work into (n-1) steps, each of which cancels the elements below the pivot of column $(\boldsymbol{a_{ij}}\ \text{pour}\ \boldsymbol{i} > \boldsymbol{j})$. At the beginning of each step, we verify that the pivot is non-zero. For step i, the pivot is $\boldsymbol{a_{ii}^{(i-1)}}$ at step (i-1).

The system in its initial state or at step (0) is given by:

$$\begin{bmatrix} a_{11} & a_{12} & a_{1n} \\ a_{21} & a_{22} \cdots & a_{2n} \\ & \vdots & \\ a_{n1} & a_{n2} \ldots & a_{nn} \end{bmatrix}^{(0)} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}^{(0)} = \begin{bmatrix} a_{1n+1} \\ a_{2n+1} \\ \vdots \\ a_{nn+1} \end{bmatrix}^{(0)}$$

First step:

We first verify that the pivot of the first step, which is $a_{ii}^{(i-1)} \neq 0 \; for \; i = 1$ i.e $a_{11}^{(0)} \neq 0$.

To cancel the element $a_{21}^{(0)}$ of the second row, we multiply the first equation by $a_{21}^{(0)}$ and divide it by $a_{11}^{(0)}$, then we take the difference of this new equation with the second. The resulting equation will replace the second one $E_2^{(1)} = E_2^{(0)} - E_1^{(0)} \frac{a_{21}^{(0)}}{a_{11}^{(0)}}$.

This operation gives $a_{21}^{(1)} = 0, \; a_{22}^{(1)} = a_{22}^{(0)} - a_{12}^{(0)} \frac{a_{21}^{(0)}}{a_{11}^{(0)}}, \; \ldots.., \; a_{2n+1}^{(1)} = a_{2n+1}^{(0)} - a_{1n+1}^{(0)} \frac{a_{21}^{(0)}}{a_{11}^{(0)}}$.

In general, we write: $a_{2j}^{(1)} = a_{2j}^{(0)} - a_{1j}^{(0)} \frac{a_{21}^{(0)}}{a_{11}^{(0)}}$ for $j = 2, n+1$

We continue this procedure with rows 3, 4, ..., for row *i* we have: $E_i^{(1)} = E_i^{(0)} - E_1^{(0)} \frac{a_{i1}^{(0)}}{a_{11}^{(0)}}$

This operation gives $a_{i1}^{(1)} = 0, \; a_{i2}^{(1)} = a_{i2}^{(0)} - a_{12}^{(0)} \frac{a_{i1}^{(0)}}{a_{11}^{(0)}}, \; \ldots.., \; a_{in+1}^{(1)} = a_{in+1}^{(0)} - a_{1n+1}^{(0)} \frac{a_{i1}^{(0)}}{a_{11}^{(0)}}$.

In general, we write: $a_{ij}^{(1)} = a_{ij}^{(0)} - a_{1j}^{(0)} \frac{a_{i1}^{(0)}}{a_{11}^{(0)}}$ for $i = 2, \mathrm{n}$ et $j = 2, n+1$

At the end of the first step, we obtain zero elements below the pivot of the first step. The system is written as:

$$\begin{bmatrix} a_{11}^{(0)} & a_{12}^{(0)} & \cdots & a_{1n}^{(0)} \\ 0 & a_{22}^{(1)} & & a_{2n}^{(1)} \\ & \vdots & & \\ 0 & a_{n2}^{(1)} & \ldots & a_{nn}^{(1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_{1n+1}^{(0)} \\ a_{2n+1}^{(1)} \\ \vdots \\ a_{nn+1}^{(1)} \end{bmatrix}$$

Second step: $a_{ii}^{(i-1)} \neq 0$ pour $i = 2$ i.e $a_{22}^{(1)} \neq 0$.

De la même façon, on obtient pour le cas général

$$a_{ij}^{(2)} = a_{ij}^{(1)} - a_{2j}^{(1)} \frac{a_{i2}^{(1)}}{a_{22}^{(1)}} \quad \text{Pour } \mathrm{i} = 3, \mathrm{n} \text{ et } j = 3, n+1$$

Step *k* : $a_{ii}^{(i-1)} \neq 0$ for $i = k$ i.e $a_{kk}^{(k-1)} \neq 0$.

For an arbitrary step k, we have:

$$a_{ij}^{(k)} = a_{ij}^{(k-1)} - a_{kj}^{(k-1)} \frac{a_{ik}^{(k-1)}}{a_{kk}^{(k-1)}} \quad \text{For } k = \overline{1, n-1}, \quad i = \overline{k+1, n} \text{ and } j = \overline{k+1, n+1}$$

At the end of the procedure, we obtain a system with an upper triangular matrix, which is written as:

$$\begin{bmatrix} a_{11}^{(0)} & a_{12}^{(0)} & \cdots & a_{1n}^{(0)} \\ 0 & a_{22}^{(1)} & & a_{2n}^{(1)} \\ & \vdots & & \\ 0 & 0 & & a_{nn}^{(n-1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_{1n+1}^{(0)} \\ a_{2n+1}^{(1)} \\ \vdots \\ a_{nn+1}^{(n-1)} \end{bmatrix}$$

The solution of this system is done by backward substitution.

5.1.2 The number of operations required for the application of the Gaussian algorithm is:

Number of multiplications and additions:

$$nm = na = \frac{n(n-1)(2n+5)}{6}$$

Number of divisions:

$$nd = \frac{n(n+1)}{2}$$

5.1.3 Applications of the Gaussian method.

a) **The determinant of a triangular matrix** is given by:

$$\det(U) = (-1)^P \prod_{i=1}^{n} u_{ii} = (-1)^P u_{11}u_{22} \dots . u_{nn}$$

With P being the number of row or column permutations performed during the application of the Gaussian algorithm.

Example: Consider the following system of equations:

$$\begin{cases} 2x + y + 2z = 10 \\ 3x + 5y + z = 16 \\ -x + 4y + 7z = 28 \end{cases}$$

1. Calculate the number of elementary operations for the Gauss method. 2. Calculate the determinant of the system's matrix. 3. Solve the system by Gaussian elimination. 4. Recalculate the determinant of the system's matrix.

b) **Simultaneous solution of multiple systems** with the same matrix A: In practice, we often encounter the case of several systems of equations that differ only in the right-hand side B. We can apply the Gaussian algorithm to the matrix A augmented by all the right-hand sides. In this way, we do the calculations only once on the matrix A, and the substitution is done with each right-hand side obtained separately.

$$\begin{bmatrix} a_{11} & a_{12} & a_{1n} \\ a_{21} & a_{22} \cdots & a_{2n} \\ & \vdots & \\ a_{n1} & a_{n2} \dots & a_{nn} \end{bmatrix} \begin{bmatrix} b_1 & c_1 & z_1 \\ b_2 & c_2 \cdots & z_2 \\ & \vdots & \\ b_n & c_n \dots & z_n \end{bmatrix}$$

c) Calculation of the inverse of a matrix:

If A is a matrix of order n, the matrix A^{-1} such that $AA^{-1} = I$ is called the inverse matrix of A.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{1n} \\ a_{21} & a_{22} \cdots & a_{2n} \\ & \vdots & \\ a_{n1} & a_{n2} \dots & a_{nn} \end{bmatrix} \text{ et } \boldsymbol{A^{-1}} = \begin{bmatrix} x_{11} & x_{12} & x_{1n} \\ x_{21} & x_{22} \cdots & x_{2n} \\ & \vdots & \\ x_{n1} & x_{n2} \dots & x_{nn} \end{bmatrix}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{1n} \\ a_{21} & a_{22} \cdots & a_{2n} \\ & \vdots & \\ a_{n1} & a_{n2} \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_{11} & x_{12} & x_{1n} \\ x_{21} & x_{22} \cdots & x_{2n} \\ & \vdots & \\ x_{n1} & x_{n2} \dots & x_{nn} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 \cdots & 0 \\ & \vdots & \\ 0 & 0 \dots & 1 \end{bmatrix}$$

Example: Consider the following matrix:

$$\begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 1 & 1 \end{bmatrix}$$

1. Use the Gauss method to calculate the inverse matrix.
2. Calculate the number of operations.

5.2. <u>Use of pivoting</u>.

In the development of the Gaussian algorithm, it was assumed that the pivot is not zero, which is not always the case. Sometimes the pivot is very small compared to the other terms or even zero, in which case we can use the technique of pivoting, either partial or total.

Partial pivoting:

In this case, we choose as the pivot the element $a_{lk}^{(k-1)}$ such that:

$$a_{lk}^{(k-1)} = \max_{i\in[k,n]} \left| a_{ik}^{(k-1)} \right|$$

$$\begin{bmatrix} a_{11} \dots & a_{1k} & a_{1n} \\ 0 \dots & \boldsymbol{a_{kk}} & \dots a_{kn} \\ & \vdots & \\ 0 \dots & \boldsymbol{a_{nk}} & \dots a_{nn} \end{bmatrix}$$

In partial pivoting, we use row permutations, which do not affect the solution of the system.

Total pivoting:

In total pivoting, the choice of the pivot is made from a submatrix including the permutation of rows and columns such that:

$$a_{lm}^{(k-1)} = \max_{i,j\in[k,n]} \left| a_{ij}^{(k-1)} \right|$$

$$\begin{bmatrix} a_{11} \dots & a_{1k} & a_{1n} \\ 0 \dots & \boldsymbol{a_{kk}} & \dots a_{kn} \\ & \vdots & \\ 0 \dots & \boldsymbol{a_{nk}} & \dots a_{nn} \end{bmatrix}$$

Example: Consider the following system:

$$\begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 1 \\ 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 9 \\ 8 \\ 7 \end{bmatrix}$$

Use the Gauss method with partial pivoting, then total pivoting, to solve the system.

<u>5.2 Thomas Algorithm TDMA</u>

In numerical methods for solving partial differential equations, we encounter matrices with three diagonals (main diagonal, sub-diagonal, and super-diagonal). This type of matrix is called tri-diagonal. The algorithm for solving this type of system is a special case of Gaussian elimination. Consider the following system with a tri-diagonal matrix:

$$\begin{pmatrix} b_1 & c_1 & & & & & \\ a_2 & b_2 & c_2 & & \cdots & & \\ & a_3 & b_3 & c_3 & & & \\ & \vdots & & & \ddots & & \vdots \\ & & & & a_{n-2} & b_{n-2} & c_{n-2} \\ & & & \cdots & a_{n-1} & b_{n-1} & c_{n-1} \\ & & & & & a_n & b_n \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{n-2} \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{n-2} \\ y_{n-1} \\ y_n \end{pmatrix}$$

We divide the first row by b_1, which gives: $1 \quad c_1/b_1 \quad \cdots \quad y_1/b_1$

We denote $\gamma_1 = c_1/b_1$ and $\beta_1 = y_1/b_1$

Next, we transform the second row by: $E_2^{(1)} = E_2^{(0)} - E_1^{(0)} a_2$ which gives :

$$0 \qquad b_2 - a_2\gamma_1 \qquad c_2 \ldots\ldots \; y_2 - a_2\beta_1$$

We divide the new second row by $b_2 - a_2\gamma_1$ which gives :

$$0 \qquad 1 \qquad c_2/(b_2 - a_2\gamma_1) \ldots\ldots \; (y_2 - a_2\beta_1)/(b_2 - a_2\gamma_1)$$

We denote $\gamma_2 = c_2/(b_2 - a_2\gamma_1)$ and $\beta_2 = (y_2 - a_2\beta_1)/(b_2 - a_2\gamma_1)$

In the same way, we continue with the third row, which gives:

$$0 \qquad 0 \qquad 1 \qquad c_3/(b_3 - a_3\gamma_2) \quad \ldots\ldots (y_3 - a_3\beta_2)/(b_3 - a_3\gamma_2)$$

We denote $\gamma_3 = c_3/(b_3 - a_3\gamma_2)$ and $\beta_3 = (y_3 - a_3\beta_2)/(b_3 - a_3\gamma_2)$

In general, for a row i, we have:

$$0 \qquad 0 \ldots..0 \qquad 1 \qquad c_i/(b_i - a_i\gamma_{i-1}) \quad \ldots\ldots (y_i - a_i\beta_{i-1})/(b_i - a_i\gamma_{i-1})$$

with $\quad \gamma_i = c_i/(b_i - a_i\gamma_{i-1}) \qquad i = \overline{2, n-1}$

and $\quad \beta_i = (y_i - a_i\beta_{i-1})/(b_i - a_i\gamma_{i-1}) \quad i = \overline{2, n}$

We continue until we obtain the following system:

$$\begin{pmatrix} 1 & \gamma_1 & & & & & \\ & 1 & \gamma_2 & & \cdots & & \\ & & 1 & \gamma_3 & & & \\ & \vdots & & & \ddots & & \vdots \\ & & & & 1 & \gamma_{n-2} & \\ & & & \cdots & & 1 & \gamma_{n-1} \\ & & & & & & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{n-2} \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \\ \beta_{n-2} \\ \beta_{n-1} \\ \beta_n \end{pmatrix}$$

The solution of the system is easily obtained by backward substitution:

$$x_n = \beta_n$$

$$x_i = \beta_i - \gamma_i x_{i+1} \quad i = \overline{n-1, 1}$$

In summary, to apply the Thomas algorithm, we calculate:

$$\begin{cases} \gamma_1 = \dfrac{c_1}{b_1} \\ \gamma_i = c_i/(b_i - a_i\gamma_{i-1}) \quad i = \overline{2, n-1} \end{cases}$$

$$\begin{cases} \beta_1 = \dfrac{y_1}{b_1} \\ \beta_i = (y_i - a_i\beta_{i-1})/(b_i - a_i\gamma_{i-1}) \quad i = \overline{2,n} \end{cases}$$

$$\begin{cases} x_n = \beta_n \\ x_i = \beta_i - \gamma_i x_{i+1} \quad i = \overline{n-1,1} \end{cases}$$

Example: Consider the following system:

$$\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 4 \\ 8 \\ 8 \end{bmatrix}$$

Use the Thomas algorithm to solve the system.