Numerical Methods for Chemical Engineers

Chapter 3: System of Linear Algebraic Equation

Morteza Esfandyari

Email: Esfandyari.morteza@yahoo.com

Mesfandyari.mihanblog.com

System of Linear Algebraic Equations

This chapter deals with the case of determining the values $x_1, x_2, \ldots, x_n$ that simultaneously satisfy a set of equations:

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

where the a's are constant coefficients, b's are constants and n is the number of equations.

Goals and Objectives

- ✓Be able to solve problems involving linear algebraic equations
- ✓Appreciate the usage of linear algebraic equations in any field of engineering
- ✓Mastering several techniques and their reliability
    - ❑Naïve Gauss elimination
    - ❑Gauss-Jordan elimination
    - ❑LU decomposition
    - ❑Gauss Siedel
    - ❑Jacobi's method
- ✓Be able to use a program to successfully solve systems of linear algebraic equations

Naïve Gauss *Elimination*

A systematic technique use to solve linear algebraic equations simultaneously with two steps:

a) Forward elimination

- the equations were manipulated to eliminate all the elements below the main diagonal of matrix A

b) Back Substitution

- the elimination step result in one equation with one unknown.
- the equation could be solved directly and the result back-substituted into one of the original equations to solve the remaining unknown.

The procedure of Naïve Gauss Elimination

Representing the linear algebraic equations in an augmented matrix form.

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + .. + a_{1n}x_n &= c_1 \\
a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + .. + a_{2n}x_n &= c_2 \\
a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + .. + a_{3n}x_n &= c_3 \\
\vdots \qquad \vdots \qquad \vdots \qquad & \quad \vdots \\
a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + .. + a_{nn}x_n &= c_n
\end{aligned}
$$

$$
\begin{bmatrix} a_{11} & a_{12} & a_{13}.. & a_{1n} \\ a_{21} & a_{22} & a_{23}.. & a_{2n} \\ a_{31} & a_{32} & a_{33}.. & a_{3n} \\ a_{n1} & a_{n2} & a_{n3}.. & a_{3n} \end{bmatrix}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_n \end{bmatrix}
=
\begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_n \end{bmatrix}
$$

$$
\left[\begin{array}{cccc:c} a_{11} & a_{12} & a_{13}.. & a_{1n} & c_1 \\ a_{21} & a_{22} & a_{23}.. & a_{2n} & c_2 \\ a_{31} & a_{32} & a_{33}.. & a_{3n} & c_3 \\ a_{n1} & a_{n2} & a_{n3}.. & a_{nn} & c_4 \end{array}\right]
\begin{array}{l} - \ (1) \\ - \ (2) \\ - \ (3) \\ - \ (n) \end{array}
$$

Label as row or eqn. (1).

Steps of Naïve Gauss Elimination (ex. 3 unknowns in 3 equations).

A) Forward elimination

a) To eliminate the first unknown, x_1, from the second through the nth row/eqn.
- row/eqn (1) is called the pivot equation, and a_{11} is called pivot element.

$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & c_1 \\ a_{21} & a_{22} & a_{23} & c_2 \\ a_{31} & a_{32} & a_{33} & c_3 \end{array}\right]\begin{array}{l} -(1) \\ -(2) \\ -(3) \end{array}$$

$$\Downarrow$$

$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & c_1 \\ & a'_{22} & a'_{23} & c'_2 \\ & a'_{32} & a'_{33} & c'_3 \end{array}\right]\begin{array}{l} -(1) \\ -(2') \\ -(3') \end{array}$$

(i) (1) x a_{21}/a_{11} $\Rightarrow$ (1a)
(ii) (2) – (1a) $\Rightarrow$ (2')
(iii) (1) x a_{31}/a_{11} $\Rightarrow$ (1b)
(iv) (3) – (1b) $\Rightarrow$ (3')

the prime ' indicates that the elements have been modified.

➢ Steps of Naïve Gauss Elimination (ex. 3 unknowns in 3 equations).

b) To eliminate the second unknown, x_2, from the third through the nth row/eqn.
- row/eqn (2') is called the pivot equation.

$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & c_1 \\ & a'_{22} & a'_{23} & c'_2 \\ & a'_{32} & a'_{33} & c'_3 \end{array}\right] \begin{array}{l} -(1) \\ -(2') \\ -(3') \end{array}$$

(i) (2') x a'_{32}/a'_{22} $\Rightarrow$ (2'a)

(ii) (3') – (2'a) $\Rightarrow$ (3")

$$\Downarrow$$

$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & c_1 \\ & a'_{22} & a'_{23} & c'_2 \\ & & a''_{33} & c''_3 \end{array}\right] \begin{array}{l} -(1) \\ -(2') \\ -(3'') \end{array}$$

the double prime " indicates that the elements have been modified twice.

Steps of Naïve Gauss Elimination (ex. 3 unknowns in 3 equations).

B) Back Substitution

From equation (3'') : $[a''_{33} \;\; c''_{33}]$ ® $a''_{33}x_3 = c''_3$

$$4 \; x_3 = c''_3/a''_{33}$$

the result x_3 can be back-substituted into eqn (2') and (1) to solve for $x_2$andx_1.

$$\left.\begin{aligned} x_2 &= (c'_2 - a'_{23}x_3)/a'_{22} \\ x_1 &= (c_1 - a_{12}x_2 - a_{13}x_3)/a_{11} \end{aligned}\right\} \text{From equation (2') and (1)}$$

Naïve Gauss Elimination

(assignment in class)

Use Naïve Gauss elimination to solve the following equations.

$$x_1 + x_2 - x_3 = -3$$
$$6x_1 + 2x_2 + 2x_3 = 2$$
$$-3x_1 + 4x_2 + x_3 = 1$$

Gauss-Jordan Elimination

Steps of Gauss-Jordan Elimination (ex. 3 unknowns in 3 equations).

a) Change the value of a_{11} to 1 and eliminate the other elements in the first column.

$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & c_1 \\ a_{21} & a_{22} & a_{23} & c_2 \\ a_{31} & a_{32} & a_{33} & c_3 \end{array}\right] \begin{array}{l} -(1) \\ -(2) \\ -(3) \end{array}$$

$$\Downarrow$$

$$\left[\begin{array}{ccc|c} 1 & a'_{12} & a'_{13} & c'_1 \\ 0 & a'_{22} & a'_{23} & c'_2 \\ 0 & a'_{32} & a'_{33} & c'_3 \end{array}\right] \begin{array}{l} -(1') \\ -(2') \\ -(3') \end{array}$$

(i) (1) x $1/a_{11}$ $\Rightarrow$ (1')
(ii) (1') x a_{21} $\Rightarrow$ (1'a)
(iii) (2) – (1'a) $\Rightarrow$ (2')
(iv) (1') x a_{31} $\Rightarrow$ (1'b)
(v) (3) – (1'b) $\Rightarrow$ (3')

the prime ' indicates that the elements have been modified.

Steps of Gauss-Jordan Elimination (ex. 3 unknowns in 3 equations).

b) Change the value of a'_{22} to 1 and eliminate the other elements in the second column.

$$\left[\begin{array}{ccc|c} 1 & a'_{12} & a'_{13} & c'_1 \\ 0 & a'_{22} & a'_{23} & c'_2 \\ 0 & a'_{32} & a'_{33} & c'_3 \end{array}\right]\begin{array}{l} -(1') \\ -(2') \\ -(3') \end{array}$$

$$\Downarrow$$

$$\left[\begin{array}{ccc|c} 1 & 0 & a''_{13} & c''_1 \\ 0 & 1 & a''_{23} & c''_2 \\ 0 & 0 & a''_{33} & c''_3 \end{array}\right]\begin{array}{l} -(1'') \\ -(2'') \\ -(3'') \end{array}$$

(i) $(2') \times 1/a'_{22} \Rightarrow (2'')$
(ii) $(2'') \times a'_{12} \Rightarrow (2''a)$
(iii) $(1') - (2''a) \Rightarrow (1'')$
(iv) $(2'') \times a'_{32} \Rightarrow (2''b)$
(v) $(3') - (2''b) \Rightarrow (3'')$

the double prime " indicates that the elements have been modified twice.

Steps of Gauss-Jordan Elimination (ex. 3 unknowns in 3 equations).

c) Change the value of a''_{33} to 1 and eliminate the other elements in the third column.

$$\left[\begin{array}{ccc:c} 1 & 0 & a''_{13} & c''_1 \\ 0 & 1 & a''_{23} & c''_2 \\ 0 & 0 & a''_{33} & c''_3 \end{array}\right] \begin{array}{l} -(1'') \\ -(2'') \\ -(3'') \end{array}$$

$$\Downarrow$$

$$\left[\begin{array}{ccc:c} 1 & 0 & 0 & c'''_1 \\ 0 & 1 & 0 & c'''_2 \\ 0 & 0 & 1 & c'''_3 \end{array}\right] \begin{array}{l} -(1''') \\ -(2''') \\ -(3''') \end{array}$$

(i) $(3'') \times 1/a''_{33} \Rightarrow (3''')$
(ii) $(3''') \times a''_{13} \Rightarrow (3'''a)$
(iii) $(1'') - (3'''a) \Rightarrow (1''')$
(iv) $(3''') \times a''_{23} \Rightarrow (3'''b)$
(v) $(2'') - (3'''b) \Rightarrow (2''')$

the triple prime 23 indicates that the elements have been modified three times.

Steps of Gauss-Jordan Elimination (ex. 3 unknowns in 3 equations).

d) The value of the unknowns can be determined directly without the back substitution step as in the naïve gauss elimination.

$$\left[\begin{array}{ccc|c} 1 & 0 & 0 & c_1''' \\ 0 & 1 & 0 & c_2''' \\ 0 & 0 & 1 & c_3''' \end{array}\right] \begin{array}{l} -(1''') \\ -(2''') \\ -(3''') \end{array} \Rightarrow \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} c_1''' \\ c_2''' \\ c_3''' \end{bmatrix}$$

$$x_1 = c_1'''$$
$$x_2 = c_2'''$$
$$x_3 = c_3'''$$

Gauss Seidel Method

The most commonly used iterative method for linear equations solving.

The linear equations were derived so that the first equation can be solved for x_1, the second can be solved for x_2 and the third can be solved for x_3.

$$
\begin{array}{l}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + .. + a_{1n}x_n = c_1 \\
a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + .. + a_{2n}x_n = c_2 \\
a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + .. + a_{3n}x_n = c_3 \\
\quad \vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad \vdots \qquad \vdots \\
a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + .. + a_{nn}x_n = c_n
\end{array}
$$

$$x_1 = \frac{c_1 - a_{12}x_2 - a_{13}x_3 - \cdots - a_{1n}x_n}{a_{11}} \qquad x_2 = \frac{c_2 - a_{21}x_1 - a_{23}x_3 - \cdots - a_{2n}x_n}{a_{22}}$$

$$x_3 = \frac{c_3 - a_{31}x_1 - a_{32}x_2 - \cdots - a_{3n}x_n}{a_{33}} \qquad x_n = \frac{c_n - a_{n2}x_2 - a_{n3}x_3 - \cdots - a_{nm}x_m}{a_{nn}}$$

Jacobi's Method

the Jacobi method is an algorithm for determining the solutions of a system of linear equations with largest absolute values in each row and column dominated by the diagonal element. Each diagonal element is solved for, and an approximate value plugged in. The process is then iterated until it converges. This algorithm is a stripped-down version of the Jacobi transformation method of matrix diagonalization.

$$x_i^{k+1} = (b_i - \sum_{j \neq i} a_{ij} x_j^k) / a_{ii}$$

k=0,1,…

Convergence Test

$$\left\| x^{k+1} - x^k \right\| \leq \varepsilon$$

Step for Gauss Seidel

$$x_1 = \frac{c_1}{a_{11}}$$

$$x_2 = \frac{(c_2 - a_{21}x_1)}{a_{22}}$$

$$x_3 = \frac{(c_3 - a_{31}x_1 - a_{32}x_2)}{a_{33}}$$

First Iteration

$$x_1 = \frac{(c_1 - a_{12}x_2 - a_{13}x_3)}{a_{11}}$$

$$x_2 = \frac{(c_2 - a_{21}x_1 - a_{23}x_3)}{a_{22}}$$

$$x_3 = \frac{(c_3 - a_{31}x_1 - a_{32}x_2)}{a_{33}}$$

Second Iteration

$$\left|\varepsilon_{a,i}\right| = \left|\frac{x_i^j - x_i^{j-1}}{x_i^j}\right| 100\% < \varepsilon_s$$

convergence criteria where j and j -1 are the present and previous iterations

Gauss Seidel

(assignment in class)

Use the Gauss Seidel method to solve the following equations ($\varepsilon_s = 5\ \%$).

$$17x_1 - 2x_2 - 3x_3 = 500$$
$$-5x_1 + 21x_2 - 2x_3 = 200$$
$$-5x_1 - 5x_2 + 22x_3 = 30$$

Gauss Seidel – assignment in class

Figure 1.0 shows a chemical process consists of 3 reactors linked by pipes. The mass flowrate of a chemical (g/s) through each pipe is equal to its concentration in each reactor, c (g/m^3) multiplied by the volume flowrate (m^3/s) of the pipe. Assume the system is at a steady state, so that the transfer into each reactor will balance the transfer out. Develop mass-balance equations for the reactors, and solve the equations simultaneously for the unknown concentrations (c_1, c_2, c_3) using Gauss-Siedel method with $\varepsilon_s = 5\%$.

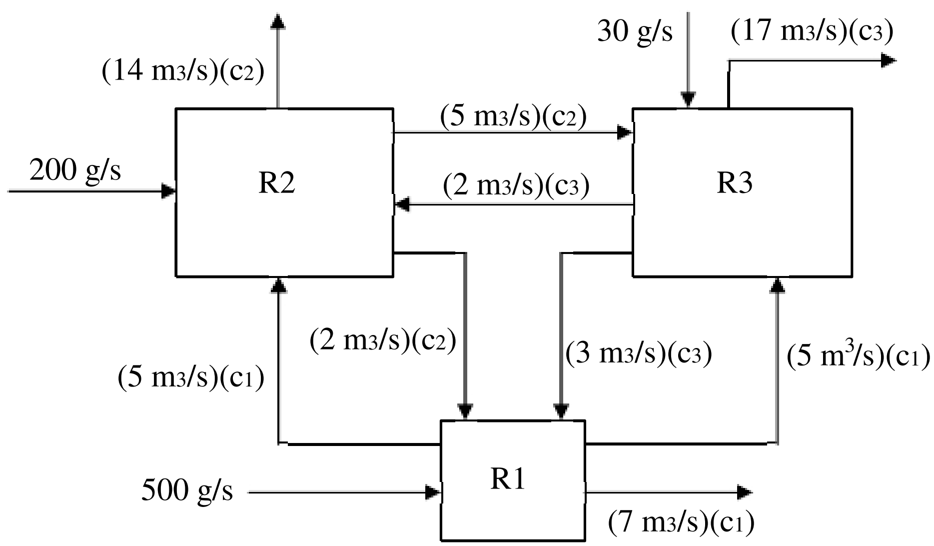

Figure 1.0


The End