

## Chapter 04.06

# Gaussian Elimination

After reading this chapter, you should be able to:

1. solve a set of simultaneous linear equations using Naïve Gauss elimination,
2. learn the pitfalls of the Naïve Gauss elimination method,
3. understand the effect of round-off error when solving a set of linear equations with the Naïve Gauss elimination method,
4. learn how to modify the Naïve Gauss elimination method to the Gaussian elimination with partial pivoting method to avoid pitfalls of the former method,
5. find the determinant of a square matrix using Gaussian elimination, and
6. understand the relationship between the determinant of a coefficient matrix and the solution of simultaneous linear equations.

### How is a set of equations solved numerically?

One of the most popular techniques for solving simultaneous linear equations is the Gaussian elimination method. The approach is designed to solve a general set of  $n$  equations and  $n$  unknowns

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

Gaussian elimination consists of two steps

1. Forward Elimination of Unknowns: In this step, the unknown is eliminated in each equation starting with the first equation. This way, the equations are *reduced* to one equation and one unknown in each equation.
2. Back Substitution: In this step, starting from the last equation, each of the unknowns is found.

### Forward Elimination of Unknowns:

In the first step of forward elimination, the first unknown,  $x_1$  is eliminated from all rows below the first row. The first equation is selected as the pivot equation to eliminate  $x_1$ . So,

to eliminate  $x_1$  in the second equation, one divides the first equation by  $a_{11}$  (hence called the pivot element) and then multiplies it by  $a_{21}$ . This is the same as multiplying the first equation by  $a_{21}/a_{11}$  to give

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

Now, this equation can be subtracted from the second equation to give

$$\left(a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right)x_2 + \dots + \left(a_{2n} - \frac{a_{21}}{a_{11}}a_{1n}\right)x_n = b_2 - \frac{a_{21}}{a_{11}}b_1$$

or

$$a'_{22}x_2 + \dots + a'_{2n}x_n = b'_2$$

where

$$\begin{aligned} a'_{22} &= a_{22} - \frac{a_{21}}{a_{11}}a_{12} \\ &\vdots \\ a'_{2n} &= a_{2n} - \frac{a_{21}}{a_{11}}a_{1n} \end{aligned}$$

This procedure of eliminating  $x_1$ , is now repeated for the third equation to the  $n^{\text{th}}$  equation to reduce the set of equations as

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n &= b_1 \\ a'_{22}x_2 + a'_{23}x_3 + \dots + a'_{2n}x_n &= b'_2 \\ a'_{32}x_2 + a'_{33}x_3 + \dots + a'_{3n}x_n &= b'_3 \\ &\vdots \\ &\vdots \\ &\vdots \\ a'_{n2}x_2 + a'_{n3}x_3 + \dots + a'_{nn}x_n &= b'_n \end{aligned}$$

This is the end of the first step of forward elimination. Now for the second step of forward elimination, we start with the second equation as the pivot equation and  $a'_{22}$  as the pivot element. So, to eliminate  $x_2$  in the third equation, one divides the second equation by  $a'_{22}$  (the pivot element) and then multiply it by  $a'_{32}$ . This is the same as multiplying the second equation by  $a'_{32}/a'_{22}$  and subtracting it from the third equation. This makes the coefficient of  $x_2$  zero in the third equation. The same procedure is now repeated for the fourth equation till the  $n^{\text{th}}$  equation to give

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n &= b_1 \\ a'_{22}x_2 + a'_{23}x_3 + \dots + a'_{2n}x_n &= b'_2 \\ a''_{33}x_3 + \dots + a''_{3n}x_n &= b''_3 \\ &\vdots \\ &\vdots \\ &\vdots \\ a''_{n3}x_3 + \dots + a''_{nn}x_n &= b''_n \end{aligned}$$

The next steps of forward elimination are conducted by using the third equation as a pivot equation and so on. That is, there will be a total of  $n - 1$  steps of forward elimination. At the end of  $n - 1$  steps of forward elimination, we get a set of equations that look like

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n &= b_1 \\ a'_{22}x_2 + a'_{23}x_3 + \dots + a'_{2n}x_n &= b'_2 \\ a''_{33}x_3 + \dots + a''_{3n}x_n &= b''_3 \\ &\vdots \\ &\vdots \\ &\vdots \\ a^{(n-1)}_{nn}x_n &= b^{(n-1)}_n \end{aligned}$$

### Back Substitution:

Now the equations are solved starting from the last equation as it has only one unknown.

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

Then the second last equation, that is the  $(n - 1)^{\text{th}}$  equation, has two unknowns:  $x_n$  and  $x_{n-1}$ , but  $x_n$  is already known. This reduces the  $(n - 1)^{\text{th}}$  equation also to one unknown. Back substitution hence can be represented for all equations by the formula

$$x_i = \frac{b_i^{(i-1)} - \sum_{j=i+1}^n a_{ij}^{(i-1)}x_j}{a_{ii}^{(i-1)}} \quad \text{for } i = n - 1, n - 2, \dots, 1$$

and

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

### Example 1

A liquid-liquid extraction process conducted in the Electrochemical Materials Laboratory involved the extraction of nickel from the aqueous phase into an organic phase. A typical set of experimental data from the laboratory is given below.

Ni aqueous phase, $a$ (g/l)	2	2.5	3
Ni organic phase, $g$ (g/l)	8.57	10	12

Assuming  $g$  is the amount of Ni in the organic phase and  $a$  is the amount of Ni in the aqueous phase, the quadratic interpolant that estimates  $g$  is given by

$$g = x_1a^2 + x_2a + x_3, \quad 2 \leq a \leq 3$$

The solution for the unknowns  $x_1$ ,  $x_2$ , and  $x_3$  is given by

$$\begin{bmatrix} 4 & 2 & 1 \\ 6.25 & 2.5 & 1 \\ 9 & 3 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ 10 \\ 12 \end{bmatrix}$$

Find the values of  $x_1$ ,  $x_2$ , and  $x_3$  using naïve Gauss elimination. Estimate the amount of nickel in the organic phase when 2.3 g/l is in the aqueous phase using quadratic interpolation.

**Solution**

**Forward Elimination of Unknowns**

Since there are three equations, there will be two steps of forward elimination of unknowns.

First step

Divide Row 1 by 4 and then multiply it by 6.25, that is, multiply Row 1 by  $6.25/4 = 1.5625$ .

$$\text{Row 1} \times (1.5625) = [6.25 \quad 3.125 \quad 1.5625] \quad [13.391]$$

Subtract the result from Row 2 to get

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 9 & 3 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 12 \end{bmatrix}$$

Divide Row 1 by 4 and then multiply it by 9, that is, multiply Row 1 by  $9/4 = 2.25$ .

$$\text{Row 1} \times (2.25) = [9 \quad 4.5 \quad 2.25] \quad [19.283]$$

Subtract the result from Row 3 to get

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & -1.25 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ -7.2825 \end{bmatrix}$$

Second step

We now divide Row 2 by  $-0.625$  and then multiply it by  $-1.5$ , that is, multiply Row 2 by  $-1.5/-0.625 = 2.4$ .

$$\text{Row 2} \times (2.4) = [0 \quad -1.5 \quad -1.35] \quad [-8.1375]$$

Subtract the result from Row 3 to get

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 0.855 \end{bmatrix}$$

**Back Substitution**

From the third equation,

$$0.1x_3 = 0.855$$

$$\begin{aligned} x_3 &= \frac{0.855}{0.1} \\ &= 8.55 \end{aligned}$$

Substituting the value of  $x_3$  in the second equation,

$$(-0.625)x_2 + (-0.5625)x_3 = -3.3906$$

$$\begin{aligned}
 x_2 &= \frac{-3.3906 - (-0.5625)x_3}{-0.625} \\
 &= \frac{-3.3906 - (-0.5625) \times 8.55}{-0.625} \\
 &= -2.27
 \end{aligned}$$

Substituting the values of  $x_2$  and  $x_3$  in the first equation,

$$\begin{aligned}
 4x_1 + 2x_2 + x_3 &= 8.57 \\
 x_1 &= \frac{8.57 - 2x_2 - x_3}{4} \\
 &= \frac{8.57 - 2 \times (-2.27) - 8.55}{4} \\
 &= 1.14
 \end{aligned}$$

Hence the solution vector is

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.14 \\ -2.27 \\ 8.55 \end{bmatrix}$$

The polynomial that passes through the three data points is then

$$\begin{aligned}
 g(a) &= x_1 a^2 + x_2 a + x_3 \\
 &= 1.14a^2 + (-2.27)a + 8.55
 \end{aligned}$$

where  $g$  is the amount of nickel in the organic phase and  $a$  is the amount of nickel in the aqueous phase.

When 2.3 g/l is in the aqueous phase, using quadratic interpolation, the estimated amount of nickel in the organic phase is

$$\begin{aligned}
 g(2.3) &= 1.14 \times (2.3)^2 + (-2.27) \times (2.3) + 8.55 \\
 &= 9.3596 \text{ g/l}
 \end{aligned}$$

### Example 2

Use Naïve Gauss elimination to solve

$$\begin{aligned}
 20x_1 + 15x_2 + 10x_3 &= 45 \\
 -3x_1 - 2.249x_2 + 7x_3 &= 1.751 \\
 5x_1 + x_2 + 3x_3 &= 9
 \end{aligned}$$

Use six significant digits with chopping in your calculations.

#### Solution

Working in the matrix form

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

**Forward Elimination of Unknowns**First step

Divide Row 1 by 20 and then multiply it by  $-3$ , that is, multiply Row 1 by  $-3/20 = -0.15$ .

$([20 \ 15 \ 10] \ [45]) \times -0.15$  gives Row 1 as

$$[-3 \ -2.25 \ -1.5] \ [-6.75]$$

Subtract the result from Row 2

$$\begin{array}{r} [-3 \ -2.249 \ 7] \ [1.751] \\ - [-3 \ -2.25 \ -1.5] \ [-6.75] \\ \hline 0 \ 0.001 \ 8.5 \ 8.501 \end{array}$$

to get the resulting equations as

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & 0.001 & 8.5 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 8.501 \\ 9 \end{bmatrix}$$

Divide Row 1 by 20 and then multiply it by 5, that is, multiply Row 1 by  $5/20 = 0.25$

$([20 \ 15 \ 10] \ [45]) \times 0.25$  gives Row 1 as

$$[5 \ 3.75 \ 2.5] \ [11.25]$$

Subtract the result from Row 3

$$\begin{array}{r} [5 \ 1 \ 3] \ [9] \\ - [5 \ 3.75 \ 2.5] \ [11.25] \\ \hline 0 \ -2.75 \ 0.5 \ -2.25 \end{array}$$

to get the resulting equations as

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & 0.001 & 8.5 \\ 0 & -2.75 & 0.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 8.501 \\ -2.25 \end{bmatrix}$$

Second step

Now for the second step of forward elimination, we will use Row 2 as the pivot equation and eliminate Row 3: Column 2.

Divide Row 2 by 0.001 and then multiply it by  $-2.75$ , that is, multiply Row 2 by  $-2.75/0.001 = -2750$ .

$([0 \ 0.001 \ 8.5] \ [8.501]) \times -2750$  gives Row 2 as

$$[0 \ -2.75 \ -23375] \ [-23377.75]$$

Rewriting within 6 significant digits with chopping

$$[0 \ -2.75 \ -23375] \ [-23377.7]$$

Subtract the result from Row 3

$$\begin{array}{r} [0 \ -2.75 \ 0.5] \ [-2.25] \\ - [0 \ -2.75 \ -23375] \ [-23377.7] \\ \hline 0 \ 0 \ 23375.5 \ 23375.45 \end{array}$$

Rewriting within 6 significant digits with chopping

$$[0 \ 0 \ 23375.5] \ [-23375.4]$$

to get the resulting equations as

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & 0.001 & 8.5 \\ 0 & 0 & 23375.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 8.501 \\ 23375.4 \end{bmatrix}$$

This is the end of the forward elimination steps.

### Back substitution

We can now solve the above equations by back substitution. From the third equation,

$$23375.5x_3 = 23375.4$$

$$\begin{aligned} x_3 &= \frac{23375.4}{23375.5} \\ &= 0.999995 \end{aligned}$$

Substituting the value of  $x_3$  in the second equation

$$0.001x_2 + 8.5x_3 = 8.501$$

$$\begin{aligned} x_2 &= \frac{8.501 - 8.5x_3}{0.001} \\ &= \frac{8.501 - 8.5 \times 0.999995}{0.001} \\ &= \frac{8.501 - 8.49995}{0.001} \\ &= \frac{0.00105}{0.001} \\ &= 1.05 \end{aligned}$$

Substituting the value of  $x_3$  and  $x_2$  in the first equation,

$$20x_1 + 15x_2 + 10x_3 = 45$$

$$\begin{aligned} x_1 &= \frac{45 - 15x_2 - 10x_3}{20} \\ &= \frac{45 - 15 \times 1.05 - 10 \times 0.999995}{20} \\ &= \frac{45 - 15.75 - 9.99995}{20} \\ &= \frac{29.25 - 9.99995}{20} \\ &= \frac{19.2500}{20} \\ &= 0.9625 \end{aligned}$$

Hence the solution is

$$[X] = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$= \begin{bmatrix} 0.9625 \\ 1.05 \\ 0.999995 \end{bmatrix}$$

Compare this with the exact solution of

$$[X] = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \\ = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

### Are there any pitfalls of the Naïve Gauss elimination method?

Yes, there are two pitfalls of the Naïve Gauss elimination method.

**Division by zero:** It is possible for division by zero to occur during the beginning of the  $n-1$  steps of forward elimination.

For example

$$5x_2 + 6x_3 = 11$$

$$4x_1 + 5x_2 + 7x_3 = 16$$

$$9x_1 + 2x_2 + 3x_3 = 15$$

will result in division by zero in the first step of forward elimination as the coefficient of  $x_1$  in the first equation is zero as is evident when we write the equations in matrix form.

$$\begin{bmatrix} 0 & 5 & 6 \\ 4 & 5 & 7 \\ 9 & 2 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 11 \\ 16 \\ 15 \end{bmatrix}$$

But what about the equations below: Is division by zero a problem?

$$5x_1 + 6x_2 + 7x_3 = 18$$

$$10x_1 + 12x_2 + 3x_3 = 25$$

$$20x_1 + 17x_2 + 19x_3 = 56$$

Written in matrix form,

$$\begin{bmatrix} 5 & 6 & 7 \\ 10 & 12 & 3 \\ 20 & 17 & 19 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 18 \\ 25 \\ 56 \end{bmatrix}$$

there is no issue of division by zero in the first step of forward elimination. The pivot element is the coefficient of  $x_1$  in the first equation, 5, and that is a non-zero number. However, at the end of the first step of forward elimination, we get the following equations in matrix form

$$\begin{bmatrix} 5 & 6 & 7 \\ 0 & 0 & -11 \\ 0 & -7 & -9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 18 \\ -11 \\ -16 \end{bmatrix}$$

Now at the beginning of the 2<sup>nd</sup> step of forward elimination, the coefficient of  $x_2$  in Equation 2 would be used as the pivot element. That element is zero and hence would create the division by zero problem.

So it is important to consider that the possibility of division by zero can occur at the beginning of any step of forward elimination.

**Round-off error:** The Naïve Gauss elimination method is prone to round-off errors. This is true when there are large numbers of equations as errors propagate. Also, if there is subtraction of numbers from each other, it may create large errors. See the example below.

### Example 3

Remember Example 2 where we used Naïve Gauss elimination to solve

$$\begin{aligned} 20x_1 + 15x_2 + 10x_3 &= 45 \\ -3x_1 - 2.249x_2 + 7x_3 &= 1.751 \\ 5x_1 + x_2 + 3x_3 &= 9 \end{aligned}$$

using six significant digits with chopping in your calculations? Repeat the problem, but now use five significant digits with chopping in your calculations.

#### Solution

Writing in the matrix form

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

#### Forward Elimination of Unknowns

##### First step

Divide Row 1 by 20 and then multiply it by  $-3$ , that is, multiply Row 1 by  $-3/20 = -0.15$ .

$$\begin{aligned} ([20 \ 15 \ 10] \ [45]) \times -0.15 &\text{ gives Row 1 as} \\ [-3 \ -2.25 \ -1.5] &\quad [-6.75] \end{aligned}$$

Subtract the result from Row 2

$$\begin{array}{r} [-3 \ -2.249 \ 7] \quad [1.751] \\ - [-3 \ -2.25 \ -1.5] \quad [-6.75] \\ \hline 0 \quad 0.001 \quad 8.5 \quad 8.501 \end{array}$$

to get the resulting equations as

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & 0.001 & 8.5 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 8.501 \\ 9 \end{bmatrix}$$

Divide Row 1 by 20 and then multiply it by 5, that is, multiply Row 1 by  $5/20 = 0.25$ .

$$\begin{array}{r} ([20 \ 15 \ 10] \ [45]) \times 0.25 \text{ gives Row 1 as} \\ [5 \ 3.75 \ 2.5] \ [11.25] \end{array}$$

Subtract the result from Row 3

$$\begin{array}{r} [5 \ 1 \ 3] \ [9] \\ - [5 \ 3.75 \ 2.5] \ [11.25] \\ \hline 0 \ -2.75 \ 0.5 \ -2.25 \end{array}$$

to get the resulting equations as

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & 0.001 & 8.5 \\ 0 & -2.75 & 0.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 8.501 \\ -2.25 \end{bmatrix}$$

### Second step

Now for the second step of forward elimination, we will use Row 2 as the pivot equation and eliminate Row 3: Column 2.

Divide Row 2 by 0.001 and then multiply it by  $-2.75$ , that is, multiply Row 2 by  $-2.75/0.001 = -2750$ .

$$\begin{array}{r} ([0 \ 0.001 \ 8.5] \ [8.501]) \times -2750 \text{ gives Row 2 as} \\ [0 \ -2.75 \ -23375] \ [-23377.75] \end{array}$$

Rewriting within 5 significant digits with chopping

$$[0 \ -2.75 \ -23375] \ [-23377]$$

Subtract the result from Row 3

$$\begin{array}{r} [0 \ -2.75 \ 0.5] \ [-2.25] \\ - [0 \ -2.75 \ -23375] \ [-23377] \\ \hline 0 \ 0 \ 23375 \ 23374 \end{array}$$

Rewriting within 6 significant digits with chopping

$$[0 \ 0 \ 23375] \ [-23374]$$

to get the resulting equations as

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & 0.001 & 8.5 \\ 0 & 0 & 23375 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 8.501 \\ 23374 \end{bmatrix}$$

This is the end of the forward elimination steps.

### **Back substitution**

We can now solve the above equations by back substitution. From the third equation,

$$23375x_3 = 23374$$

$$\begin{aligned} x_3 &= \frac{23374}{23375} \\ &= 0.99995 \end{aligned}$$

Substituting the value of  $x_3$  in the second equation

$$0.001x_2 + 8.5x_3 = 8.501$$

$$\begin{aligned}
 x_2 &= \frac{8.501 - 8.5x_3}{0.001} \\
 &= \frac{8.501 - 8.5 \times 0.99995}{0.001} \\
 &= \frac{8.501 - 8.499575}{0.001} \\
 &= \frac{8.501 - 8.4995}{0.001} \\
 &= \frac{0.0015}{0.001} \\
 &= 1.5
 \end{aligned}$$

Substituting the value of  $x_3$  and  $x_2$  in the first equation,

$$\begin{aligned}
 20x_1 + 15x_2 + 10x_3 &= 45 \\
 x_1 &= \frac{45 - 15x_2 - 10x_3}{20} \\
 &= \frac{45 - 15 \times 1.5 - 10 \times 0.99995}{20} \\
 &= \frac{45 - 22.5 - 9.9995}{20} \\
 &= \frac{22.5 - 9.9995}{20} \\
 &= \frac{12.5005}{20} \\
 &= \frac{12.500}{20} \\
 &= 0.625
 \end{aligned}$$

Hence the solution is

$$\begin{aligned}
 [X] &= \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \\
 &= \begin{bmatrix} 0.625 \\ 1.5 \\ 0.99995 \end{bmatrix}
 \end{aligned}$$

Compare this with the exact solution of

$$[X] = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

### What are some techniques for improving the Naïve Gauss elimination method?

As seen in Example 3, round off errors were large when five significant digits were used as opposed to six significant digits. One method of decreasing the round-off error would be to use more significant digits, that is, use double or quad precision for representing the numbers. However, this would not avoid possible division by zero errors in the Naïve Gauss elimination method. To avoid division by zero as well as reduce (not eliminate) round-off error, Gaussian elimination with partial pivoting is the method of choice.

### How does Gaussian elimination with partial pivoting differ from Naïve Gauss elimination?

The two methods are the same, except in the beginning of each step of forward elimination, a row switching is done based on the following criterion. If there are  $n$  equations, then there are  $n-1$  forward elimination steps. At the beginning of the  $k^{\text{th}}$  step of forward elimination, one finds the maximum of

$$|a_{kk}|, |a_{k+1,k}|, \dots, |a_{nk}|$$

Then if the maximum of these values is  $|a_{pk}|$  in the  $p^{\text{th}}$  row,  $k \leq p \leq n$ , then switch rows  $p$  and  $k$ .

The other steps of forward elimination are the same as the Naïve Gauss elimination method. The back substitution steps stay exactly the same as the Naïve Gauss elimination method.

### Example 4

In the previous two examples, we used Naïve Gauss elimination to solve

$$20x_1 + 15x_2 + 10x_3 = 45$$

$$-3x_1 - 2.249x_2 + 7x_3 = 1.751$$

$$5x_1 + x_2 + 3x_3 = 9$$

using five and six significant digits with chopping in the calculations. Using five significant digits with chopping, the solution found was

$$\begin{aligned} [X] &= \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \\ &= \begin{bmatrix} 0.625 \\ 1.5 \\ 0.99995 \end{bmatrix} \end{aligned}$$

This is different from the exact solution of

$$[X] = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$= \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Find the solution using Gaussian elimination with partial pivoting using five significant digits with chopping in your calculations.

**Solution**

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

**Forward Elimination of Unknowns**

Now for the first step of forward elimination, the absolute value of the first column elements below Row 1 is

$$|20|, |-3|, |5|$$

or

$$20, 3, 5$$

So the largest absolute value is in the Row 1. So as per Gaussian elimination with partial pivoting, the switch is between Row 1 and Row 1 to give

$$\begin{bmatrix} 20 & 15 & 10 \\ -3 & -2.249 & 7 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 1.751 \\ 9 \end{bmatrix}$$

Divide Row 1 by 20 and then multiply it by  $-3$ , that is, multiply Row 1 by  $-3/20 = -0.15$ .

$$([20 \ 15 \ 10] \ [45]) \times -0.15 \text{ gives Row 1 as}$$

$$[-3 \ -2.25 \ -1.5] \ [-6.75]$$

Subtract the result from Row 2

$$\begin{array}{r} [-3 \ -2.249 \ 7] \ [1.751] \\ - [-3 \ -2.25 \ -1.5] \ [-6.75] \\ \hline 0 \ 0.001 \ 8.5 \ 8.501 \end{array}$$

to get the resulting equations as

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & 0.001 & 8.5 \\ 5 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 8.501 \\ 9 \end{bmatrix}$$

Divide Row 1 by 20 and then multiply it by 5, that is, multiply Row 1 by  $5/20 = 0.25$ .

$$([20 \ 15 \ 10] \ [45]) \times 0.25 \text{ gives Row 1 as}$$

$$[5 \ 3.75 \ 2.5] \ [11.25]$$

Subtract the result from Row 3

$$\begin{array}{r} [5 \ 1 \ 3] \ [9] \\ - [5 \ 3.75 \ 2.5] \ [11.25] \\ \hline 0 \ -2.75 \ 0.5 \ -2.25 \end{array}$$

to get the resulting equations as

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & 0.001 & 8.5 \\ 0 & -2.75 & 0.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ 8.501 \\ -2.25 \end{bmatrix}$$

This is the end of the first step of forward elimination.

Now for the second step of forward elimination, the absolute value of the second column elements below Row 1 is

$$|0.001|, |-2.75|$$

or

$$0.001, 2.75$$

So the largest absolute value is in Row 3. So Row 2 is switched with Row 3 to give

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & -2.75 & 0.5 \\ 0 & 0.001 & 8.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ -2.25 \\ 8.501 \end{bmatrix}$$

Divide Row 2 by  $-2.75$  and then multiply it by  $0.001$ , that is, multiply Row 2 by  $0.001/-2.75 = -0.00036363$ .

$$([0 \quad -2.75 \quad 0.5] \quad [-2.25]) \times -0.00036363 \text{ gives Row 2 as}$$

$$[0 \quad 0.00099998 \quad -0.00018182] \quad [0.00081816]$$

Subtract the result from Row 3

$$\begin{array}{r} [0 \quad 0.001 \quad 8.5] \quad [8.501] \\ - [0 \quad 0.00099998 \quad -0.00018182] \quad [0.00081816] \\ \hline 0 \quad 0 \quad 8.50018182 \quad 8.50018184 \end{array}$$

Rewriting within 5 significant digits with chopping

$$[0 \quad 0 \quad 8.5001] \quad [8.5001]$$

to get the resulting equations as

$$\begin{bmatrix} 20 & 15 & 10 \\ 0 & -2.75 & 0.5 \\ 0 & 0 & 8.5001 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 45 \\ -2.25 \\ 8.5001 \end{bmatrix}$$

**Back substitution**

$$8.5001x_3 = 8.5001$$

$$x_3 = \frac{8.5001}{8.5001} \\ = 1$$

Substituting the value of  $x_3$  in Row 2

$$-2.75x_2 + 0.5x_3 = -2.25$$

$$x_2 = \frac{-2.25 - 0.5x_3}{-2.75} \\ = \frac{-2.25 - 0.5 \times 1}{-2.75}$$

$$\begin{aligned}
 &= \frac{-2.25 - 0.5}{-2.75} \\
 &= \frac{-2.75}{-2.75} \\
 &= 1
 \end{aligned}$$

Substituting the value of  $x_3$  and  $x_2$  in Row 1

$$\begin{aligned}
 20x_1 + 15x_2 + 10x_3 &= 45 \\
 x_1 &= \frac{45 - 15x_2 - 10x_3}{20} \\
 &= \frac{45 - 15 \times 1 - 10 \times 1}{20} \\
 &= \frac{45 - 15 - 10}{20} \\
 &= \frac{30 - 10}{20} \\
 &= \frac{20}{20} \\
 &= 1
 \end{aligned}$$

So the solution is

$$\begin{aligned}
 [X] &= \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \\
 &= \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}
 \end{aligned}$$

This, in fact, is the exact solution. By coincidence only, in this case, the round-off error is fully removed.

### Can we use Naïve Gauss elimination methods to find the determinant of a square matrix?

One of the more efficient ways to find the determinant of a square matrix is by taking advantage of the following two theorems on a determinant of matrices coupled with Naïve Gauss elimination.

#### Theorem 1:

Let  $[A]$  be a  $n \times n$  matrix. Then, if  $[B]$  is a  $n \times n$  matrix that results from adding or subtracting a multiple of one row to another row, then  $\det(A) = \det(B)$  (The same is true for column operations also).

**Theorem 2:**

Let  $[A]$  be a  $n \times n$  matrix that is upper triangular, lower triangular or diagonal, then

$$\begin{aligned}\det(A) &= a_{11} \times a_{22} \times \dots \times a_{ii} \times \dots \times a_{nn} \\ &= \prod_{i=1}^n a_{ii}\end{aligned}$$

This implies that if we apply the forward elimination steps of the Naïve Gauss elimination method, the determinant of the matrix stays the same according to Theorem 1. Then since at the end of the forward elimination steps, the resulting matrix is upper triangular, the determinant will be given by Theorem 2.

**Example 5**

Find the determinant of

$$[A] = \begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$$

**Solution**

Remember in Example 1, we conducted the steps of forward elimination of unknowns using the Naïve Gauss elimination method on  $[A]$  to give

$$[B] = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$

According to Theorem 2

$$\begin{aligned}\det(A) &= \det(B) \\ &= 25 \times (-4.8) \times 0.7 \\ &= -84.00\end{aligned}$$

**What if I cannot find the determinant of the matrix using the Naïve Gauss elimination method, for example, if I get division by zero problems during the Naïve Gauss elimination method?**

Well, you can apply Gaussian elimination with partial pivoting. However, the determinant of the resulting upper triangular matrix may differ by a sign. The following theorem applies in addition to the previous two to find the determinant of a square matrix.

**Theorem 3:**

Let  $[A]$  be a  $n \times n$  matrix. Then, if  $[B]$  is a matrix that results from switching one row with another row, then  $\det(B) = -\det(A)$ .

**Example 6**

Find the determinant of

$$[A] = \begin{bmatrix} 10 & -7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix}$$

**Solution**

The end of the forward elimination steps of Gaussian elimination with partial pivoting, we would obtain

$$[B] = \begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.002 \end{bmatrix}$$

$$\begin{aligned} \det(B) &= 10 \times 2.5 \times 6.002 \\ &= 150.05 \end{aligned}$$

Since rows were switched once during the forward elimination steps of Gaussian elimination with partial pivoting,

$$\begin{aligned} \det(A) &= -\det(B) \\ &= -150.05 \end{aligned}$$

**Example 7**

Prove

$$\det(A) = \frac{1}{\det(A^{-1})}$$

**Solution**

$$\begin{aligned} [A][A]^{-1} &= [I] \\ \det(A A^{-1}) &= \det(I) \\ \det(A)\det(A^{-1}) &= 1 \\ \det(A) &= \frac{1}{\det(A^{-1})} \end{aligned}$$

If  $[A]$  is a  $n \times n$  matrix and  $\det(A) \neq 0$ , what other statements are equivalent to it?

1.  $[A]$  is invertible.
2.  $[A]^{-1}$  exists.
3.  $[A][X] = [C]$  has a unique solution.
4.  $[A][X] = [0]$  solution is  $[X] = [\vec{0}]$ .
5.  $[A][A]^{-1} = [I] = [A]^{-1}[A]$ .

**Key Terms:**

*Naïve Gauss Elimination*

*Partial Pivoting*

*Determinant*

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**SIMULTANEOUS LINEAR EQUATIONS**

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Topic	Gaussian Elimination
Summary	Textbook notes of Gaussian Elimination
Major	Chemical Engineering
Authors	Autar Kaw
Date	November 8, 2012
Web Site	<a href="http://numericalmethods.eng.usf.edu">http://numericalmethods.eng.usf.edu</a>

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