2. Linear Algebraic Equations

Many physical systems yield simultaneous algebraic equations when mathematical functions are required to satisfy several conditions simultaneously. Each condition results in an equation that contains known coefficients and unknown variables. A system of ‘n’ linear equations can be expressed as

$$AX = C \tag{1}$$

Where ‘A’ is a ‘n x n’ coefficient matrix, ‘C’ is ‘nx1’ right hand side vector, and ‘X’ is an ‘n x 1’ vector of unknowns.

Gauss elimination, Gauss-Jordan and LU decomposition methods are direct elimination methods.

2.1 Gauss elimination method:

This method comprises of two steps:

(i) Forward elimination of unknowns

(ii) Back substitution

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots\ldots\ldots\ldots \quad + a_{1n}x_n = C_1 \qquad (2a)$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots\ldots\ldots\ldots \quad + a_{2n}x_n = C_2 \qquad (2b)$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \ldots\ldots\ldots\ldots \quad + a_{3n}x_n = C_3 \qquad (2c)$$

....

....

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \ldots\ldots\ldots\ldots \quad + a_{nn}x_n = C_n \qquad (2n)$$

Forward elimination of unknowns:

The first step is designed to reduce the set of equations to an upper triangular system.

Multiply Eq. (2a) by a_{21}/a_{11}. This gives

$$a_{21}x_1 + (a_{21}/a_{11})\,a_{12}x_2 + (a_{21}/a_{11})\,a_{13}x_3 + \ldots \qquad (3)$$
$$\ldots\ldots\ldots + (a_{21}/a_{11})\,a_{1n}x_n = (a_{21}/a_{11})c_1$$

Modify Eq. (2b) by subtracting Eq. (3) from Eq. (2b). Now the equation is in the form

$$(0) + \left(a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right)x_2 + \ldots + \left(a_{2n} - \frac{a_{21}}{a_{11}}a_{1n}\right)xn = c_2 - \frac{a_{21}}{a_{11}}c_1 \qquad (4a)$$

Or $\quad a'_{22}x_2 + \ldots\ldots\ldots\ldots\ldots + a'_{2n}x_n = c'_2 \qquad (4b)$

Prime indicates that the elements have been changed from their original values.

Similarly, Eq. (2c) can be modified by multiplying

Eq. (2a) with $\frac{a_{31}}{a_{11}}$ and subtracting from Eq. (2c)

and the nth equation can be modified by multiplying

Eq. (2a) by $\frac{a_{n1}}{a_{11}}$ and subtract from Eq. (2n)

Following are the modified system of equations

$$a_{11} x_1 + a_{12} x_2 + a_{13} x_3 + \ldots\ldots + a_{1n} x_n = c_1 \quad (5a)$$

$$a'_{22} x_2 + a'_{23} x_3 + \ldots\ldots + a'_{2n} x_n = c'_2 \quad (5b)$$

$$a'_{32} x_2 + a'_{33} x_3 + \ldots\ldots + a'_{3n} x_n = c'_3 \quad (5c)$$

....

....

$$a'_{n2} x_2 + a'_{n3} x_3 + \ldots\ldots + a'_{nn} x_n = c'_n \quad (5n)$$

Repeat the above process to eliminate the second unknown from Eq. (5c) to the last equation. This process yield

$$a_{11}x_1 + a_{12}x_2 + a_{13}\,x_3 + \ldots\ldots + a_{1n}\,x_n = c_1 \qquad (6a)$$

$$a'_{22}x_2 + a'_{23}x_3 + \ldots \quad + a'_{2n}x_n = c'_2 \qquad (6b)$$

$$a''_{33}\,x_3 + \ldots \quad + a''_{3n}x_n = c''_3 \qquad (6c)$$

$$\ldots\ldots\ldots\ldots\ldots\ldots \qquad \ldots\ldots\ldots\ldots\ldots\ldots$$

$$a''_{n3}\,x_3 + \ldots\ldots + a''_{nn}\,x_n = c''_n \qquad (6n)$$

Double prime indicates that the elements have been modified twice.

The problem can be continued to eliminate x_{n-1} term from n^{th} equation. At this stage the system of equation has been transformed to upper triangular system as shown below.

$$a_{11} x_1 + a_{12} x_2 + a_{13} x_3 + \ldots\ldots\ldots\ldots\ldots\ldots + a_{1n} x_n = c_1$$

$$a'_{22} x_2 + a'_{23} x_3 + \ldots\ldots\ldots\ldots\ldots\ldots + a'_{2n} x_n = c'_2$$

$$a''_{33} x_3 + \ldots\ldots\ldots\ldots\ldots\ldots + a''_{3n} x_n = c''_3$$

$$\ldots\ldots\ldots \qquad \ldots\ldots\ldots\ldots$$

$$a^{(n-1)}_{nn} x_n = c^{(n-1)}_n$$

- (7)

The above step can be algorithmically written as

$$a_{ij}^{k} = a_{ij}^{(k-1)} - \frac{a_{i,k-1}^{(k-1)}}{a_{k-1,k-1}^{(k-1)}} a_{k-1,j}^{(k-1)} \qquad (8)$$

$$c_{i}^{k} = c_{i}^{(k-1)} - \frac{a_{i,k-1}^{(k-1)}}{a_{k-1,k-1}^{(k-1)}} c_{k-1}^{(k-1)} \qquad (9)$$

k= 2, 3, 4, 5,………………… , n (10a)

i= k, k+1, k+2, ………………., n (10b)

j= k, k+1, k+2, ………………., n (10c)

Back substitution:

The solution x can be obtained by considering the Eqn. (7) and writing for x_n

$$x_n = \frac{c_n^{(n-1)}}{a_{nn}^{(n-1)}} \qquad (11)$$

This can be back substituted into (n-1)th equation to solve for x_{n-1}. The procedure for evaluating the remaining x's can be symbolically represented as

$$x_i = \frac{c^{(i-1)}{}_i - \sum_{j=i+1}^{n} a_{ij}^{(i-1)} x_j}{a^{(i-1)}{}_{ii}} \qquad (12)$$

for i = n–1, n–2, n–3, ……., 1

Example2.1:

Solve using Gauss elimination method

$$\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 2 \\ 4 \end{Bmatrix}$$

Forward elimination:

Elimination of 1st unknown x_1 :

Multiply first row by 1/2 and subtract to second row; no operation is required on third row since $a_{31}^{(1)}$ = 0 already:

$$\begin{bmatrix} 2 & 1 & 0 \\ 0 & 3/2 & 1 \\ 0 & 1 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 3/2 \\ 4 \end{Bmatrix}$$

Elimination of 2nd unknown x_2 :

Multiply 2nd row by 2/3 and subtract from third row;

$$\begin{bmatrix} 2 & 1 & 0 \\ 0 & 3/2 & 1 \\ 0 & 0 & 1/3 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 3/2 \\ 3 \end{Bmatrix}$$

Backward substitution:

$(1/3)\, x_3 = 3$ $\qquad x_3 = 9$

$(3/2)\, x_2 + x_3 = 3/2$ $\qquad x_2 = -5$

$2x_1 + x_2 = 1$ $\qquad x_1 = 3$

On the method:

No of multiplication and divisions:

$$\frac{N^3 + 3N^2 - N}{3} \approx \frac{N^3}{3}$$

No of additions and subtractions:

$$\frac{N^3 + 3N^2 - N}{3} \approx \frac{N^3}{3} \qquad (13)$$

2.2 Pitfalls of elimination methods:

Although many systems of equations can be solved by Gauss-elimination method, there are some pitfalls with these methods.

(a) Division by Zero.

During both the elimination and backward substitution phase, it is possible that a division by zero could occur.

$$
\begin{aligned}
2x_2 + 3x_3 &= 8 \\
4x_1 + 6x_2 + 7x_3 &= -3 \\
2x_1 + x_2 + 6x_3 &= 5
\end{aligned}
$$

Normalization of first row (a_{21}/a_{11}) involves division by $a_{11} = 0$. Problems also can arise when a coefficient is very close to zero. Pivoting techniques (discussed later) can partially avoid these problems.

(b) Round-off errors:

Computer can support a limited number of significant digits, round off errors can occur and it is important to consider this, when evaluating the results. This is particularly important when large number of equations are to be solved.

(c) Ill –conditioned system:

Well conditioned systems are those where a small change in one or more of the coefficients results in a similar small change in solution.

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- ***Ill conditioned*** systems are those where a small change in coefficients result in large changes in the solution. Ill conditioning also can be interpreted as a wide range of answers can approximately satisfying the equations. As round-off errors can induce small changes in the coefficients, these artificial changes can lead to large solution errors for ill-conditioned systems, as illustrated in the following example.

Example 2.2:

Solve the following system of equations.

(a) $x_1 + 2x_2 = 10$

$1.1x_1 + 2x_2 = 10.4$

(b) $x_1 + 2x_2 = 10$

$1.05x_1 + 2x_2 = 10.4$

Compare the results.

Solution:

Using Cramer's rule

$$x_1 = \frac{\begin{pmatrix} c_1 & a_{12} \\ c_2 & a_{22} \end{pmatrix}}{\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}} = \frac{c_1 a_{22} - a_{12} c_2}{a_{11} a_{22} - a_{12} a_{21}} \quad (1)$$

$$x_2 = \frac{\begin{pmatrix} a_{11} & c_1 \\ a_{21} & c_2 \end{pmatrix}}{\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}} = \frac{a_{11} c_2 - c_1 a_{21}}{a_{11} a_{22} - a_{12} a_{21}} \quad (2)$$

Now the solution to Example 2.2(a) can be written as

$$x_1 = \frac{10(2) - 2(10.4)}{1(2) - 2(1.1)} = 4 \qquad x_2 = \frac{1(10.4) - 1.1(10)}{1(2) - 2(1.1)} = 3$$

Now, Example 2.2(b) is with a small change of the coefficient a_{21} from 1.1 to 1.05. This will cause a dramatic change in results

$$x_1 = \frac{10(2) - 2(10.4)}{1(2) - 2(1.05)} = 8 \qquad x_2 = \frac{1(10.4) - 1.05(10)}{1(2) - 2(1.1)} = 1$$

Substituting the values $x_1 = 8$ and $x_2 = 1$ into Example 2.2(a)

$$8+2(1) = 10 \quad \approx 10$$

$$1.1(8) + 2(1) = 10.8 \approx 10.4$$

Although, $x_1=8$ and $x_2=1$ is not the true solution to the original problem, the error check is too close enough to possibly mislead you into believing that your solutions are adequate. This situation can mathematically be characterized in following general form.

$$a_{11} x_1 + a_{12} x_2 = c_1 \qquad (3)$$

$$a_{21} x_1 + a_{22} x_2 = c_2 \qquad (4)$$

From the above two equations, x_2 can be written as

$$x_2 = -\frac{a_{11}}{a_{12}} x_1 + \frac{c_1}{a_{12}} \quad (5) \qquad x_2 = -\frac{a_{21}}{a_{22}} x_1 + \frac{c_2}{a_{22}} \quad (6)$$

If the slopes are nearly equal, $\frac{a_{11}}{a_{12}} \approx \frac{a_{21}}{a_{22}}$

Or cross multiplying,

$$a_{11}\, a_{22} \approx a_{21} a_{12}$$

Which can also expressed as

$$a_{11}\, a_{22} - a_{21} a_{12} \approx 0 \qquad (7)$$

Now, recall $a_{11}a_{22} - a_{12}a_{21}$ is the determinant of a two dimensional system.

Hence, a general conclusion can be that an ill-conditioned system is one with a determinant close to zero.

Effect of scale on the determinant:

Example 2.3:

Evaluate the determinant for the following system.

(a) $3x_1 + 2x_2 = 18$ (b) $x_1 + 2x_2 = 10$

$-x_1 + 2x_2 = 2$ $1.1x_1 + 2x_2 = 10.4$

(c) Repeat (b) but with Eqs. Multiplied by10

Solution:

(a) Determinant, $D = 3(2) - (-1)(2) = 8$

So, it is well conditioned system.

(b) Determinant, $D = 1(2) - (1.1)(2) = -0.2$

It is ill conditioned system.

(c) Now multiply equations in (b) with 10

$$10x_1 + 20x_2 = 100$$

$$11x_1 + 20x_2 = 104$$

Determinant, $D = 10(20) - (11)(20) = -20$

The above example shows the magnitude of the coefficients interjects a scale effect that complicates the relationship between system condition and determinant size.

One way to partially circumvent this difficulty is **to scale** the equations so that the **maximum element in any row is equal to 1**.

Example 2.4:

Scale the equation in example 2.3

(a) $x_1 + 0.667x_2 = 6$

$-0.5x_1 + x_2 = 1$

D=1(1) – (0.5)(0.667) = 1.333

(b) For ill conditioned system

$0.5x_1 + x_2 = 5$

$0.55x_1 + x_2 = 5.2$

D = 0.5(1) – 0.55(1) = –0.05

(c) $0.5x_1 + x_2 = 5$

$0.55x_1 + x_2 = 5.2$

Scaling changes the system to the same form as in (b) and the determinant is also -0.05. Thus, the scale effect is removed.

2.3 Techniques for improving solutions:

(a) Use of extended precision:

The simplest remedy for ill conditioning is to use more significant digits in the computations, also called extended precision or high precision. The price is higher computational costs.

(b) Pivoting:

(i) Problems occur when a pivot element is zero because the normalization step leads to division by zero.

(ii) Problems may also arise when a pivot element is close to zero. When the magnitude of pivot element is small compared to the other elements, then round off errors can occur.

Partial pivoting: Before the rows are normalized, they can be swapped so that the largest element is brought to the pivot element. This is called partial pivoting.

Complete pivoting: If both columns and rows are searched for the largest element and then switched to the pivot position, it is called complete pivoting.

Example 2.5 (Partial pivoting)

Use Gauss elimination to solve

$$0.0003x_1 + 3.0000x_2 = 2.0001$$

$$1.0000x_1 + 1.0000x_2 = 1.0000$$

Solution:

Multiply first equation by (1/0.0003) yields

$$x_1 + 10000x_2 = 6667$$

Eliminating x_1 from the second equation

$$-9999x_2 = -6666$$

Or $\quad x_2 = 2/3$

Substituting back into the first equation

$$x_1 = \frac{2.0001 - 3(2/3)}{0.0003}$$

Due to subtractive cancellation, the result is very sensitive to the number of significant digits

Significant digits	x_2	x_1	% relative error for x_1
3	0.667	-3.00	1099
4	0.6667	0.0000	100
5	0.66667	0.30000	10
6	0.666667	0.330000	1
7	0.6666667	0.3330000	0.1

Now, if the equations in Example 2.5 are solved in reverse order, the row with largest pivot element is normalized.

$$1.0000x_1 + 1.0000x_2 = 1.0000$$

$$0.0003x_1 + 3.0000x_2 = 2.0001$$

Elimination and substitution yield $x_2 = 2/3$

and

$$x_1 = \frac{1 - (2/3)}{1}$$

This is much sensitive to the number of significant digits.

Significant digits	x_2	x_1	% relative error for x_1
3	0.667	0.333	0.1
4	0.6667	0.3333	0.01
5	0.66667	0.33333	0.001
6	0.666667	0.333333	0.0001
7	0.6666667	0.3333333	0.00001

(c) Scaling:

When some coefficients are very large than others, round off errors can occur. The coefficients can be standardized by scaling.

Solve the following set of equations by Gauss elimination and pivoting strategy.

$$2x_1 + 100{,}000\ x_2 = 100{,}000$$

$$x_1 + x_2 = 2$$

(a) Without scaling, forward elimination

$$2x_1 + 100{,}000\ x_2 = 100{,}000$$

$$-\ 49{,}999\ x_2 = -\ 49{,}998$$

By back substitution

$$x_2 = 1.00$$

$$x_1 = 0.00$$

(b) Scaling transform the original equation to

$$0.00002\, x_1 + x_2 = 1$$

$$x_1 + x_2 = 2$$

Put the greater value on the diagonal (pivoting)

$$x_1 + x_2 = 2$$

$$0.00002\, x_1 + x_2 = 1$$

Forward elimination yields

$$x_1 + x_2 = 2$$

$$0.99998\, x_2 = 0.99996$$

Solving $x_1 = x_2 = 1$

Scaling leads to correct answer.

(c) Pivot, but retain the original coefficients

$$x_1 + x_2 = 2$$

$$2x_1 + 100{,}000x_2 = 100{,}000$$

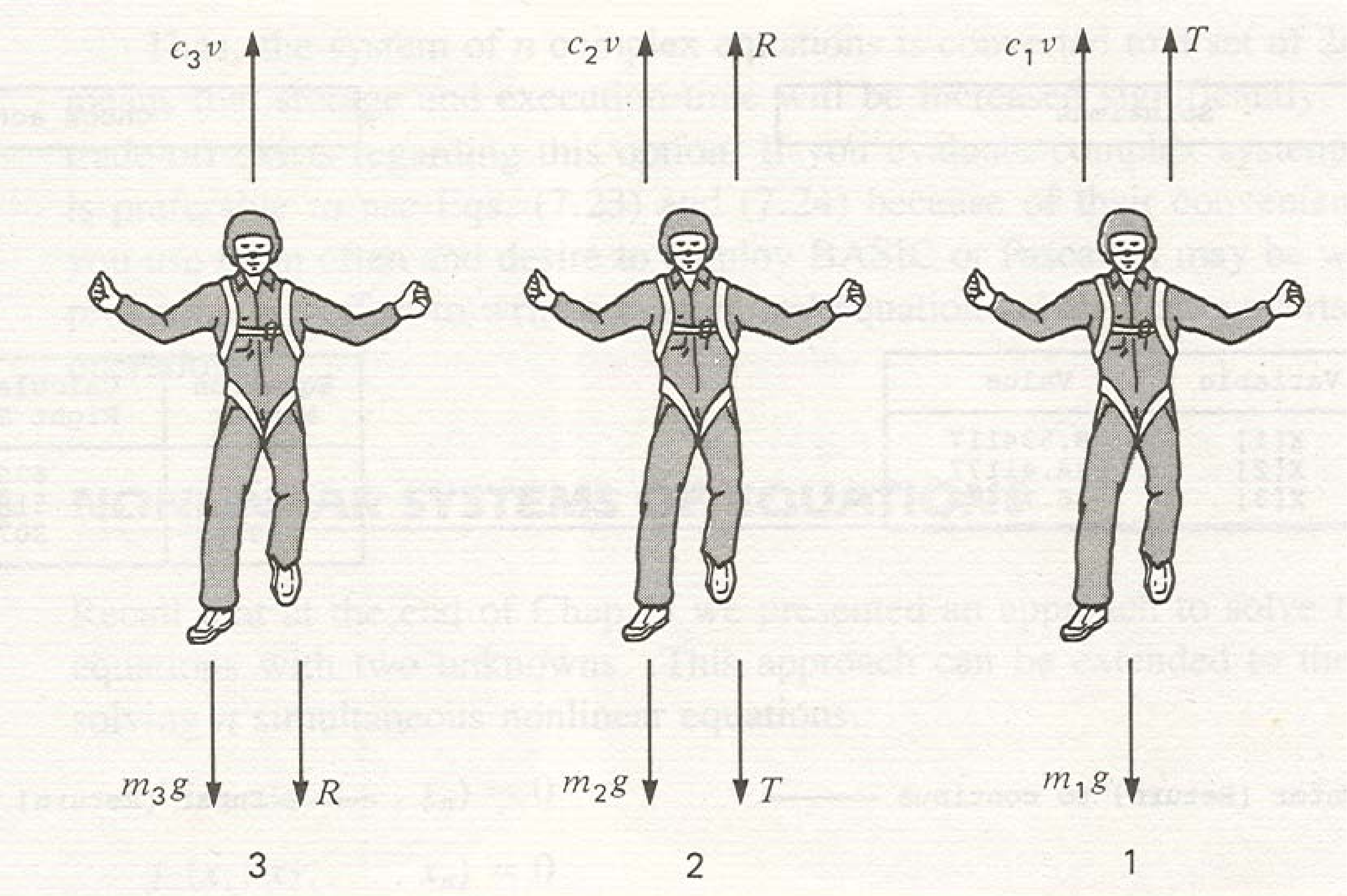
Solving we get $x_1 = x_2 = 1$

From the above results, we can observe that scaling is useful in determining whether pivoting is necessary, but the equations themselves did not require scaling to arrive at a correct result.

Example 2.6:

A team of three parachutists is connected by a weightless cord shown in figure, while free-falling at a velocity of 5m/s. Calculate the tension in each section of cord and the acceleration of the team, given the following data.

Parachutist	Mass, kg	Drag coefficient, kg/s
1	70	10
2	60	14
3	40	17



The free body diagram of each of the three parachutists is shown in the figure

Using Newton's second law

$m_1g - T - c_1v = m_1a$; $m_1a + T = m_1g - c_1v$

$m_2g + T - c_2v - R = m_2a$; $m_2a - T + R = m_2g - c_2v$

$m_3g - c_3v + R = m_3a$; $m_3a - R = m_3g - c_3v$

The three unknowns are a, T and R.

Solving

$$\begin{pmatrix} 70 & 1 & 0 \\ 60 & -1 & 1 \\ 40 & 0 & -1 \end{pmatrix}\begin{pmatrix} a \\ T \\ R \end{pmatrix} = \begin{pmatrix} 636.7 \\ 518.6 \\ 307.4 \end{pmatrix}$$

$a = 8.604 \text{ m/s}^2$

$T = 34.42 \text{ N}$

$R = 36.78 \text{ N}$

2.4. L U Decomposition Methods:

Consider the system of equations

$$[A]\{X\} = \{C\} \qquad (1)$$

Rearranging

$$[A]\{X\} - \{C\} = 0 \qquad (2)$$

Suppose that Eq. (1) can be re expressed as an upper triangle with 1 as diagonal elements.

$$\begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix} = \begin{Bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \end{Bmatrix} \qquad (3)$$

It is similar to the manipulation that occurs in the first step of Gauss elimination. Eq. (3) can be expressed as

$$[U]\ \{X\} - \{D\} = 0 \qquad (4)$$

Assume that there is a lower diagonal matrix

$$[L] = \begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \qquad (5)$$

[L] has the property that when Eqn. (4) is pre-multiplied by it, Eqn. (2) is the result.

i.e., $[L]\{[U]\{X\} - \{D\}\} = [A]\{X\} - \{C\}$ (6)

From the matrix algebra,

$[L][U] = [A]$ (7)

And $[L]\{D\} = \{C\}$ (8)

Eqn. (7) is referred to as LU decomposition of [A].

2.5. Crout Decomposition:

Gauss elimination involves two major steps: Forward elimination and backward substitution. Forward elimination step comprises the bulk of the computational effort. Most efforts have focused on economizing this step and separating it from the computations involving the right-hand-side vector. One of the most improved methods is called Crout decomposition.

$$[L]\,[U] = [A]$$

For a 4 X 4 matrix

$$\begin{bmatrix} l_{11} & 0 & 0 & 0 \\ l_{21} & l_{22} & 0 & 0 \\ l_{31} & l_{32} & l_{33} & 0 \\ l_{41} & l_{42} & l_{43} & l_{44} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} & u_{14} \\ 0 & 1 & u_{23} & u_{24} \\ 0 & 0 & 1 & u_{34} \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \quad (9)$$

1. Multiply rows of [L] with first column of [U] and equate with RHS

$l_{11} = a_{11}$ $\qquad$ $l_{21} = a_{21}$

$l_{31} = a_{31}$ $\qquad$ $l_{41} = a_{41}$

Symbolically $l_{i1} = a_{i1}$ for i = 1, 2,….,n (10)

First column of [L] is merely the first column of [A].

2. Multiply first row of [L] by the columns of [U] and equate with RHS

$l_{11} = a_{11}$ $\quad$ $l_{11}u_{12} = a_{12}$

$l_{11}u_{13} = a_{13}$ $\quad$ $l_{11}u_{14} = a_{14}$

or

$$u_{12} = \frac{a_{12}}{l_{11}} \qquad u_{13} = \frac{a_{13}}{l_{11}} \qquad u_{14} = \frac{a_{14}}{l_{11}}$$

Symbolically

$$u_{1j} = \frac{a_{1j}}{l_{11}}$$ for j = 2, 3, ……, n (11)

3. Similar operations are repeated to evaluate remaining column of [L] and the rows of [U]. Multiply second through fourth rows of [L] by second column of [U], to get

$$l_{21}u_{12} + l_{22} = a_{22}$$

$$l_{31}u_{12} + l_{32} = a_{32}$$

$$l_{41}u_{12} + l_{42} = a_{42}$$

Solving for l_{22}, l_{32} and l_{42} and representing symbolically

$$l_{i2} = a_{i2} - l_{i1}\, u_{12} \qquad \text{for } i = 2, 3, \ldots\ldots\ldots, n \qquad (12)$$

4. The remaining unknowns on the 2nd row of [U] can be evaluated by multiplying the second row of [L] by the third and fourth columns of [U] to give

$$l_{21}u_{13} + l_{22}u_{23} = a_{23}$$

$$l_{21}u_{14} + l_{22}u_{24} = a_{24}$$

which can be solved for

$$u_{23} = \frac{a_{23} - l_{21}u_{13}}{l_{22}} \qquad u_{24} = \frac{a_{24} - l_{21}u_{14}}{l_{22}}$$

which can be expressed symbolically as

$$u_{2j} = \frac{a_{2j} - l_{21}u_{1j}}{l_{22}} \quad \text{for } j = 3, 4, \ldots\ldots\ldots\ldots, n \qquad (13)$$

5. The process can be repeated to evaluate the other elements. General formulae that result are

$l_{i3} = a_{i3} - l_{i1}u_{13} - l_{i2}u_{23}$ for i = 3,4,……………,n (14)

$$u_{3j} = \frac{a_{3j} - l_{31}u_{1j} - l_{32}u_{2j}}{l_{33}}$$ for j = 4,5, …………….,n (15)

$l_{i4} = a_{i4} - l_{i1}u_{14} - l_{i2}u_{24} - l_{i3}u_{34}$ for i = 4,5, …………….,n (16)

and so forth.

Inspection of Eqn. (10) through (16) leads to the following concise formulae for implementing the method.

$l_{i1} = a_{i1}$ for i = 1, 2, 3, ……………,n (17)

$$u_{1j} = \frac{a_{1j}}{l_{11}}$$ for j = 2, 3, ……………,n (18)

For j = 2, 3, ……., n – 1,

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj}$$ for i = j, j + 1, …………,n (19)

$$u_{jk} = \frac{a_{jk} - \sum_{i=1}^{j-1} l_{ji} u_{ik}}{l_{jj}}$$ for k = j + 1, j + 2…………,n (20)

and

$$l_{nn} = a_{nn} - \sum_{k=1}^{n-1} l_{nk} u_{kn} \quad (21)$$

Back substitution step:

In Gauss elimination, the transformations involved in forward elimination are simultaneously performed on the coefficient matrix [A] and the right hand side vector {C}.

In Crout's method, once the original matrix is decomposed, [L] and [U] can be employed to solve for {X}. This is accomplished in two steps.

Step1:

Determine {D} for a particular {C} by forward substitution.

$$d_1 = \frac{c_1}{l_{11}} \qquad (22)$$

$$d_i = \frac{c_i - \sum_{j=1}^{i-1} l_{ij} d_j}{l_{ii}} \quad \text{for } i = 2,3,4,\ldots, n \qquad (23)$$

Step 2:

Eqn.(4) can be used to compute ‘X’ by back substitution

$$x_n = d_n \qquad (24)$$

$$x_i = d_i - \sum_{j=i+1}^{n} u_{ij} x_j$$

for i = n—1, n—2,…,1 (25)

Example 2.7

Solve the following system of equations by Crout's LU decomposition method.

$$2x_1 - 5x_2 + x_3 = 12$$

$$-x_1 + 3x_2 - x_3 = -8$$

$$3x_1 - 4x_2 + 2x_3 = 16$$

Solution:

According to Eq.(17), the first column of [L] is identical to the first column of [A]:

$l_{11} = 2$ $\quad$ $l_{21} = -1$ $\quad$ $l_{31} = 3$

Eqn.(18) can be used to compute the first row of [U]:

$$u_{12} = \frac{a_{12}}{l_{11}} = \frac{-5}{2} = -2.5$$

$$u_{13} = \frac{a_{13}}{l_{11}} = \frac{1}{2} = 0.5$$

The second column of [L] is computed with Eqn.(19)

$$l_{22} = a_{22} - l_{21}\, u_{12} = 3 - (-1)\,(-2.5) = 0.5$$

$$l_{32} = a_{32} - l_{31}\, u_{12} = -4 - (3)\,(-2.5) = 3.5$$

Eqn. (20) is used to compute the last element of [U],

$$u_{23} = \frac{a_{23} - l_{21} u_{13}}{l_{22}} = \frac{-1 - (-1)(0.5)}{0.5} = -1$$

and Eqn.(21) can be employed to determine the last element of [L],

$$l_{33} = a_{33} - l_{31} u_{13} - l_{32} u_{23} = 2 - 3(0.5) - 3.5(-1) = 4$$

Thus, the LU decomposition is

$$[L] = \begin{bmatrix} 2 & 0 & 0 \\ -1 & 0.5 & 0 \\ 3 & 3.5 & 4 \end{bmatrix} \qquad [U] = \begin{bmatrix} 1 & -2.5 & 0.5 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix}$$

It can be easily verified that the product of these two matrices is equal to the original matrix [A].

Then,

$$\begin{bmatrix} 2 & 0 & 0 \\ -1 & 0.5 & 0 \\ 3 & 3.5 & 4 \end{bmatrix} \begin{Bmatrix} d_1 \\ d_2 \\ d_3 \end{Bmatrix} = \begin{Bmatrix} 12 \\ -8 \\ 6 \end{Bmatrix}$$

The forward substitution procedure of Eqn. (22) and (23) can be used to solve for

$$d_1 = \frac{c_1}{l_{11}} = \frac{12}{2} = 6 \quad d_2 = \frac{c_2 - l_{21} d_1}{l_{22}} = \frac{-8 - (-1)6}{0.5} = -4$$

$$d_3 = \frac{c_3 - l_{31} d_1 - l_{32} d_2}{l_{33}} = \frac{16 - 3(+6) - 3.5(-4)}{4} = 3$$

The second step is to solve Eqn. (4), which for the present problem has the value.

$$\begin{bmatrix} 1 & -2.5 & 0.5 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 6 \\ -4 \\ 3 \end{Bmatrix}$$

The back substitution procedure of Eqs. (24) and (25) can be used to solve for

$x_3 = d_3 = 3$

$x_2 = d_2 - u_{23}\, x_3 = -4 - (-1)\, 3 = -1$

$x_1 = d_1 - u_{12}\, x_2 - u_{13}\, x_3 = 6 - (-2.5)(-1) - 0.5(3) = 2$

These values can be verified by substituting them into original equations.

$$2x_1 - 5x_2 + x_3 = 12$$

$$2(2)-5(-1)+(3) = 12$$

Thus the value are verified.

2.6. Cholesky's Decomposition

Many engineering application yield symmetric coefficient matrix. i.e., $a_{ij} = a_{ji}$ for all i and j. In other words $[A] = [A]^T$. They offer computational advantages because only half the storage is needed and in most cases, only half the computational time is required for their solution. One of the most popular approaches is Cholesky decomposition.

$$A = [B][B]^T \qquad (1)$$

In Eq.(1) resulting triangular factors are the transpose of each other.

$$\begin{bmatrix} a_{11} & & sym \\ a_{21} & a_{22} & \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} b_{11} & 0 & 0 \\ b_{21} & b_{22} & 0 \\ b_{31} & b_{32} & b_{33} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ 0 & b_{22} & b_{23} \\ 0 & 0 & b_{33} \end{bmatrix} \quad (2)$$

Because of the symmetry, it is sufficient if we consider the six elements shown in the matrix [A].

Expanding the matrices, the relationship between [A] and [B] takes the form of the following.

$$a_{11} = (b_{11})^2$$

$$a_{12} = b_{11} b_{12}$$

$$a_{13} = b_{11}\, b_{13}$$

$$a_{22} = (b_{12})^2 + (b_{22})^2$$

$$a_{23} = b_{12}\, b_{13} + b_{22}\, b_{23}$$

$$a_{33} = b_{13}^2 + b_{23}^2 + b_{33}^2$$

$$b_{11} = \sqrt{a_{11}}$$

$$b_{12} = \frac{a_{12}}{b_{11}}$$

$$b_{13} = \frac{a_{13}}{b_{11}}$$

$$b_{22} = \sqrt{a_{22} - b_{12}^2}$$

$$b_{23} = \frac{a_{23} - b_{21} b_{13}}{b_{22}} \qquad (3)$$

$$b_{33} = \sqrt{a_{33} - b_{13}^2 - b_{23}^2}$$

Hence the elements of matrix [B] can be determined by the general formulae

$$b_{kk} = \sqrt{a_{kk} - \sum_{j=1}^{k-1} b_{kj}^2}$$

$$b_{ki} = \frac{a_{ki} - \sum_{j=1}^{i-1} b_{ij}\, b_{kj}}{b_{ii}}$$

When $[A] = [B]\,[B]^T$, then

$$[B]\,[B]^T \{x\} = \{f\} \qquad (4)$$

Pre-multiplying both sides by $[B]^{-1}$

We have $[B]^T \{x\} = [B]^{-1}\{f\}$ (5)

Let $[B]^{-1} \{f\} = \{y\}$

or $f = [B]\,\{y\}$ (6)

Since { f } and [B] are known, { y } can be computed by forward substitution

$$\begin{bmatrix} b_{11} & 0 & 0 \\ b_{21} & b_{22} & 0 \\ b_{31} & b_{32} & b_{33} \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix} = \begin{Bmatrix} f_1 \\ f_2 \\ f_3 \end{Bmatrix} \qquad (7)$$

$f_1 = b_{11} y_1$

$$y_1 = \frac{f_1}{b_{11}}$$

$f_2 = b_{21} y_1 + b_{22} y_2$

$$y_2 = \frac{f_2 - b_{21} y_1}{b_{22}} \qquad (8)$$

$f_3 = b_{31} y_1 + b_{32} y_2 + b_{33} y_3$

$$y_3 = \frac{f_3 - b_{31} y_1 - b_{32} y_2}{b_{33}}$$

or symbolically,

$$y_1 = \frac{f_1}{b_{11}}$$

$$y_i = \frac{f_i - \sum_{k=1}^{i-1} b_{ik} y_k}{b_{ii}} \; or \; \frac{f_i - \sum_{k=1}^{i-1} b_{ki} y_k}{b_{ii}}$$ as $b_{ik} = b_{ki}$ (9)

having computed {y}, {x} can be computed by back substitution as following.

$[B]^T \{x\} = \{y\}$ (10)

$$\begin{bmatrix} b_{11} & b_{12} & b_{13} \\ 0 & b_{22} & b_{23} \\ 0 & 0 & b_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \end{Bmatrix} \quad (11)$$

Using the method of backward substitution *{x}* can be determined (i.e.)

$$x_n = \frac{y_n}{b_{nn}} \quad (12)$$

$$x_i = \frac{y_i - \sum_{k=i+1}^{n} b_{ik} x_k}{b_{ii}} \quad (13)$$

2.7. Gauss-Seidel Method

This is a method of successive approximations. The unknown variables are assumed to have zero values to start with. More and more correct values are then obtained in subsequent iterations.

Example:

Solve the following system of equations by Gauss-Seidel iteration.

$$10x_1 + 2x_2 + x_3 = 9$$
$$2x_1 + 20x_2 - 2x_3 = -44$$
$$-2x_1 + 3x_2 + 10x_3 = 22$$

Solution:

$$x_1 = \frac{(9 - 2x_2 - x_3)}{10} \qquad (1)$$

$$x_2 = \frac{(-44 - 2x_1 + 2x_3)}{20} \qquad (2)$$

$$x_3 = \frac{(22 + 2x_1 - 3x_2)}{10} \qquad (3)$$

or

$$x_i = \frac{B - \sum A_{ij} x_j}{A_{ii}}$$ for i = 1 to n, j = 1 to n except i.

Where B is right hand side matrix

A is coefficient matrix.

To start with let $x^{(0)}_1 = x^{(0)}_2 = x^{(0)}_3 = 0$. Substituting

$x^{(0)}_2 = x^{(0)}_3 = 0$ in Eqn. (1), we get $x^{(1)}_1 = 0.90$

$$x_1^{(1)} = 0.90 \qquad x_2^{(0)} = x_3^{(0)} = 0$$

Substituting $x_1^{(1)} = 0.90$ and $x_3^{(0)} = 0$ in Eq.(2) we get $x_2 = -2.29$

$$x_1^{(1)} = 0.90 \quad x_2^{(1)} = -2.20 - 0.90 = -2.29 \quad x_3^{(0)} = 0$$

Substitute already calculated x_2 and x_1 in Eq.(3) we get $x_3 = 3.07$.

$$x_1^{(1)} = 0.90 \quad x_2^{(1)} = -2.29 \quad x_3^{(1)} = 2.20 + 0.18 + 0.69 = 3.07$$

Note that new values of x_1 are used in place of old values as soon as they are available. This method converges faster.

The values of {X} for different iterations are tabulated below:

Iteration	0	1	2	3	4
x_1	0	0.90	1.05	1.00	1.00
x_2	0	-2.29	-2.00	-2.00	-2.00
x_3	0	3.07	3.01	3.00	3.00

We can note that there is no variation in {X} values from 3rd to 4th iteration up to second decimal. Hence iterations are stopped. It is possible to get accuracy for more decimal places as required.

SYSTEMS OF NONLINEAR EQUATIONS

$$x^2 + xy = 10 \quad \text{and} \quad y + 3xy^2 = 57$$

are two simultaneous nonlinear equations with two unknowns, x and y. They can be expressed in the form

$$u(x, y) = x^2 + xy - 10 = 0 \qquad (1a)$$

$$v(x, y) = y + 3xy^2 - 57 = 0 \qquad (1b)$$

Thus, the solution would be the values of x and y that make the functions u(x, y) and v(x, y) equal to zero. Solution method (i) one – point iteration and (ii) Netwon – Raphson

(i) One point iteration for Nonlinear System

Problem statement: Use one–point iteration to determine the roots of Eq.(1). Note that a correct pair of roots is x = 2 and y = 3. Initiate the computation with guesses of x = 1.5 and y = 3.5.

Solution: Equation (1a) can be solved for

$$x_{i+1} = \frac{10 - x_i^2}{y_i} \qquad (2a)$$

and Eq (1b) can be solved for

$$y_{i+1} = 57 - 3x_i y_i^2 \qquad (2b)$$

Note that we will drop the subscripts for the remainder of the example.

On the basis of the initial guesses, Eq (2a) can be used to determine a new value of x:

$$x = \frac{10 - (1.5)^2}{3.5} = 2.21429$$

This result and the value of y = 3.5 can be substituted into Eq. (2b) to determine a new value of y:

y = 57 – 3(2.21429) (3.5)2 = - 24.37516

Thus, the approach seems to be diverging. This behavior is even more pronounced on the second iteration

$$x = \frac{10 - \left(2.21429\right)^2}{-24.37516} = -0.20910$$

$$y = 57 - 3(-0.20910)(-24.37516)^2 = 429.709$$

Obviously, the approach is deteriorating.

Now we will repeat the computation but with the original equations set up in a different format. For example, an alternative formulation of Eq. (1a) is

$$x = \sqrt{10 - xy}$$

and of Eq.(1b) is

$$y = \sqrt{\frac{57 - y}{3x}}$$

Now the results are more satisfactory:

$$x = \sqrt{10 - 1.5(3.5)} = 2.17945$$

$$y = \sqrt{\frac{57 - 3.5}{3(2.17945)}} = 2.86051$$

$$x = \sqrt{10 - 2.17945(2.86051)} = 1.94053$$

$$y = \sqrt{\frac{57 - 2.86051}{3(1.94053)}} = 3.04955$$

$$x = \sqrt{10 - 1.94053(3.04955)} = 2.02046$$

$$y = \sqrt{\frac{57 - 3.04955}{3(2.0246)}} = 2.98340$$

Thus, the approach is converging on the true values of $x = 2$ and $y = 3$.

***Shortcoming of simple one – point iteration*:** Its convergence often depends on the manner in which the equations are formulated. Additionally, divergence can occur if the initial guesses are insufficiently close to the true solution.

$$\left|\frac{\partial u}{\partial x}\right| + \left|\frac{\partial v}{\partial x}\right| < 1 \quad and \quad \left|\frac{\partial u}{\partial y}\right| + \left|\frac{\partial v}{\partial y}\right| < 1$$

These criteria are so restrictive that one – point iteration is rarely used in practice

(ii) Newton – Raphson

$$f(x_{i+1}) = f(x_i) + \left(x_{i+1} - x_i\right) f'(x_i) \qquad (3)$$

where x_i is the initial guess at the root and x_{i+1} is the point at which the slope intercepts the x axis. At this intercept, $f(x_{i+1})$ by definition equals zero and Eq. (3) can be rearranged to yield

$$x_{i+1} = x_i - \frac{f\left(x_i\right)}{f'\left(x_i\right)} \qquad (4)$$

which is the single – equation form of the Newton–Raphson method.

The multiequation form is derived in an identical fashion.

$$u_{i+1} = u_i + (x_{i+1} - x_i)\frac{\partial u_i}{\partial x} + (y_{i+1} - y_i)\frac{\partial u_i}{\partial y} \quad (5a)$$

and

$$v_{i+1} = v_i + (x_{i+1} - x_i)\frac{\partial v_i}{\partial x} + (y_{i+1} - y_i)\frac{\partial v_i}{\partial y} \quad (5b)$$

Just as for the single-equation version, the root estimate corresponds to the points at which u_{i+1} and v_{i+1} equal zero. For this situation, Eq. (5) can be rearranged to give

$$\frac{\partial u_i}{\partial x} x_{i+1} + \frac{\partial u_i}{\partial y} y_{i+1} = -u_i + x_i \frac{\partial u_i}{\partial x} + y_i \frac{\partial u_i}{\partial y} \quad (6a)$$

and

$$\frac{\partial v_i}{\partial x} x_{i+1} + \frac{\partial v_i}{\partial y} y_{i+1} = -v_i + x_i \frac{\partial v_i}{\partial x} + y_i \frac{\partial v_i}{\partial y} \quad (6b)$$

Because all values subscripted with *i*'s are known (they correspond to the latest guess or approximation), the only unknowns are x_{i+1} and y_{i+1}. Thus, Eq. (6) is a set of two linear equations with two unknowns. Consequently, algebraic manipulations (for example, Cramer's rule) can be employed to solve for

$$x_{i+1} = x_i - \frac{u_i \frac{\partial v_i}{\partial y} - v_i \frac{\partial u_i}{\partial y}}{\frac{\partial u_i}{\partial x}\frac{\partial v_i}{\partial y} - \frac{\partial u_i}{\partial y}\frac{\partial v_i}{\partial x}} \qquad (7a)$$

and

$$y_{i+1} = y_i + \frac{u_i \frac{\partial v_i}{\partial x} - v_i \frac{\partial u_i}{\partial x}}{\frac{\partial u_i}{\partial x}\frac{\partial v_i}{\partial y} - \frac{\partial u_i}{\partial y}\frac{\partial v_i}{\partial x}} \qquad (7b)$$

The denominator of each of these equations is formally referred to as the determinant of the *Jacobian* of the system.

Equation (7) is the two-equation version of the Newton – Raphson method.

Example: Roots of Simultaneous Nonlinear Equations

Problem Statement: Use the multiple – equation Netwon – Raphon method to determine roots of Eq. (1). Note that a correct pair of roots is $x = 2$ and $y = 3$. Initiate the computation with guesses of $x = 1.5$ and $y = 3.5$.

Solution: First compute the partial derivatives and evaluate them at initial guesses

$$\frac{\partial u_0}{\partial x} = 2x + y = 2(1.5) + 3.5 = 6.5$$

$$\frac{\partial u_0}{\partial y} = x = 1.5$$

$$\frac{\partial v_0}{\partial x} = 3y^2 = 3(3.5)^2 = 36.75$$

$$\frac{\partial v_0}{\partial y} = 1 + 6xy = 1 + 6(1.5)(3.5) = 32.5$$

Thus, the determinant of the Jacobian for the first iteration is

6.5(32.5) – 1.5 (36.75) = 156.125

The values of the functions can be evaluated at the initial guesses as

$u_0 = (1.5)^2 + 1.5\,(3.5) - 10 = -2.5$

$v_0 = 3.5 + 3\,(1.5)\,(3.5)^2 - 57 = 1.625$

These values can be substituted into Eq. (7) to give

$$x_1 = 1.5 - \frac{-2.5(32.5) - 1.625(6.5)}{156.125} = 2.03603$$

and

$$y_1 = 3.5 - \frac{-2.5(36.75) - 1.625(6.5)}{156.125} = 2.84388$$

Thus, the result are converging on the true values of $x_1 = 2$ and $y_1 = 3$. The computation can be repeated until an acceptable accuracy is obtained.

The general case of solving *n* simultaneous nonlinear equations

$$f_1 (x_1, x_2, \ldots\ldots.., x_n) = 0$$

$$f_2 (x_1, x_2,\ldots\ldots.., x_n) = 0 \qquad (8)$$

$$\vdots$$

$$f_n (x_1, x_2, \ldots\ldots.., x_n) = 0$$

The solution of this system consists of the set of x values that simultaneously result in all the equations equaling zero.

A Taylor series expansion is written for each equation. For example, for the l^{th} equation

$$f_{l,i+1} = f_{l,i} + \left(x_{1,i+1} - x_{1,i}\right)\frac{\partial f_{l,i}}{\partial x_1} + \left(x_{2,i+1} - x_{2,i}\right)\frac{\partial f_{l,i}}{\partial x_2}$$

$$+ \ldots\ldots + \left(x_{n,i+1} - x_{n,i}\right)\frac{\partial f_{l,i}}{\partial x_n} \qquad (9)$$

where the first subscript, *l*, represents the equation or unknown and the second subscript denotes whether the value or function in question is at the present value (*i*) or at the next value (*i* +1).

Equations of the form of (9) are written for each of the original nonlinear equations. Then, as was done in deriving Eq. (6) from (5) , all $f_{l,i+1}$ terms are set to zero as would be the case at the root and Eq. (9) can be written as

$$- f_{l,i} + x_{1,i}\frac{\partial f_{l,i}}{\partial x_1} + x_{2,i}\frac{\partial f_{l,i}}{\partial x_2} + \ldots\ldots\ldots + x_{n,i}\frac{\partial f_{l,i}}{\partial x_n}$$

$$= x_{l,i+1}\frac{\partial f_{l,i}}{\partial x_1} + x_{2,i+1}\frac{\partial f_{l,i}}{\partial x_2} + \ldots\ldots\ldots + x_{n,i+1}\frac{\partial f_{l,i}}{\partial x_n} \qquad (10)$$

Notice that the only unknowns in Eq. (10) are the $x_{l,i+1}$ terms on the right – hand side. All other quantities are located at the present value (i) and, thus, are given at any iteration. Consequently, the set of equations generally represented Eq. (10) (that is, with l = 1,2,……,n) constitutes a set of linear simultaneous equations that can be solved by methods elaborated.

Matrix notation can be employed to express Eq. (10) concisely. The partial derivatives can be expressed as

$$[Z]=\begin{bmatrix} \frac{\partial f_{1,i}}{\partial x_1} & \frac{\partial f_{1,i}}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial f_{1,i}}{\partial x_n} \\ \frac{\partial f_{2,i}}{\partial x_1} & \frac{\partial f_{2,i}}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial f_{2,i}}{\partial x_n} \\ . & . & & . \\ . & . & & . \\ . & . & & . \\ \frac{\partial f_{n,i}}{\partial x_1} & \frac{\partial f_{n,i}}{\partial x_2} & \cdots\cdots\cdots & \frac{\partial f_{n,i}}{\partial x_n} \end{bmatrix} \tag{11}$$

The initial and final values can be expressed in vector form as

$$\{X_i\}^T = [x_{1,i} \;\; x_{2,i} \ldots\ldots . x_{n,i} \;\;]$$

$$and$$

$$\{X_{i+1}\}^T = [x_{1,i+1} \;\; x_{2,i+1} \ldots\ldots . x_{n,i+1} \;\;]$$

Finally , the function values at *i* can be expressed as

$$\{F_i\}^T = [f_{1,i} \;\; f_{2,i} \ldots\ldots . f_{n,i} \;\;]$$

Using these relationships, Eq. (10) can be represented concisely as

$$[Z]\{X_{i+1}\} = \{W_i\} \qquad (12)$$

where

$$\{W_i\} = -\{F_i\} + [Z]\{X_i\}$$

Equation (12) can be solved using a technique such as Gauss elimination. This process can be repeated iteratively to obtain refined estimates.

It should be noted that there are two major shortcomings to the forgoing approach. First, Eq. (12) is often inconvenient to evaluate. Therefore, variations of the Newton Raphson approach have been developed to circumvent this dilemma.

The second shortcoming of the multiequation Newton – Raphson method is that excellent initial guesses are usually required to unsure convergence.