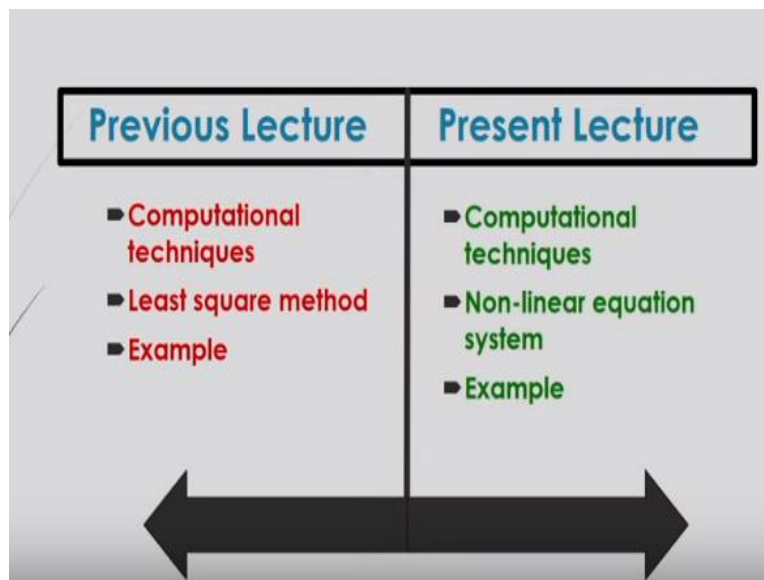


**Basic Principles and Calculations in Chemical Engineering**  
**Prof. S. K. Majumder**  
**Chemical Engineering Department**  
**Indian Institute of Technology-Guwahati**

**Lecture - 30**  
**Non-Linear Algebraic Equation System**

Welcome to massive open online course on Basic Principles and Calculations in Chemical Engineering. So we are discussing about computational techniques in module 10. And under this module in this lecture, we will discuss about nonlinear algebraic equation system and how to solve those nonlinear equation.

**(Refer Slide Time: 00:55)**



In the previous lecture we have described the least square method how to fit a linear single equation with experimental data and how to analyze the error of that fitting data with the you know that proposed equation we have discussed with example. So here also we will describe about that, how to solve that nonlinear equation system.

If suppose any nonlinear equation is coming based on the material balance equation or energy balance equation for a particular chemical engineering process, how to solve those. First of all you have to know the basic principle of that solving nonlinear equation.

**(Refer Slide Time: 01:34)**

## Nonlinear Independent Equations

$$\left. \begin{array}{l} f_1(x_1, \dots, x_n) = 0 \\ f_2(x_1, \dots, x_n) = 0 \\ \dots\dots\dots \\ f_n(x_1, \dots, x_n) = 0 \end{array} \right\} \begin{array}{l} \checkmark \\ f(x) = 0 \\ \underline{\underline{\quad}} \end{array}$$

Each function  $f(x_1, \dots, x_n)$  corresponds to a nonlinear function containing one or more of the variable whose values are unknown.

You know that there are you know several nonlinear equations will be coming based on that, you know material balance of chemical engineer processes. There you will see a set of a nonlinear equation like this here as shown in the slides here like  $f_1$  into  $x_1, \dots, x_n$ . That will be equals to 0. This is one nonlinear equation as a function of variables like  $x_1, x_n$ .

And another equation like  $f_2$  as a function of again those you know independent variables of  $x_1$  to  $x_n$ . And we can see that similarly there may be more than two equations will coming in the you know chemical engineering process for its analysis based on the material balance equation and after that we can you know recognize these set of nonlinear equation as a you know  $f(x)$  that will be equals to 0 like this.

Now each function here in the slides that  $f$  as a function of that independent variables of  $x_1$  to  $x_n$  that corresponds to a nonlinear function. Of course, that will contains one or more of the variables whose you know values are unknown which will be you know calculated by a certain principle.

**(Refer Slide Time: 03:08)**

## The major general methods of solving systems of nonlinear equations

- ▀ **Successive Substitution:**
    - ▀ Wegstein Acceleration
    - ▀ Dominant Eigenvalues Acceleration
  - ▀ **Differential – Homotopy:**
    - ▀ Continuation
    - ▀ Discrete
- ▀ **Newton (mostly used):**
    - ▀ Quasi-Newton
    - ▀ Newton-Raphson
    - ▀ Secant
    - ▀ Levenberg- Marquardt
  - ▀ **Regula-falsi method**
  - ▀ **Spreadsheet solution**
  - ▀ **Graphical solution**

Now there are you know major general you know methods of solving those nonlinear equation systems like you know some are you know successive substitution techniques, some are you know differential homotopy technique, some are Newton's, you know mostly used that method like Quasi-Newton, Newton-Raphson method, even Secant method, even Levenberg-Marquardt you know method.

Some other techniques also available like you know graphical solution even Regula-falsi method you know spreadsheet solution like this. So here we will discuss about that Newton method which are mostly used to solve that nonlinear equation.

(Refer Slide Time: 03:56)

### Solving Single variable non-linear function

- ▀ **Spreadsheet solution**

Estimate the solution of equation  $x = \exp(-2x)$  using spread sheet

Solution

x	$f(x) = x - \exp(-2x) = 0$
0.1	-0.718730753
0.2	-0.470320046
0.3	-0.248811636
0.426156	-2.73E-04
0.5	0.132120559
0.6	0.298805788
0.7	0.453403036
0.8	0.598103482
0.9	0.734701112
1	0.864664717
1.1	0.989196842
1.2	1.109282047
1.3	1.225726422
1.4	1.339189937

So here solving a single variable nonlinear equation how to solve first we have to express. There you will see that if we have the spreadsheet solution like this here,

based on that you know nonlinear equation function. In this case, let us consider that you have to you know estimate the solution of equation like  $x$  will be equals to exponent of  $-2x$  using a spreadsheet.

Now in this case, you will see that the equation here  $x$  is equal to exponent of  $-2x$  is totally you know that nonlinear equation where you will see in the both sides of this equation you know having this unknown variables like  $x$  here, you have to find out what should be the value of  $x$  so that this equation will satisfy based on that you know unknown variables there.

Now in this case you have to you know solve this equation based on spreadsheet like what is that you have to assume you know that variables here  $x$  and after substitution of that variables of that assumption value and what should be the value in you know that in left hand side and the right hand side will be coming based on which you will see that if you keep on changing that value of variables.

This you know deviation of this left hand side and right hand side will be you know coming to reduced or maybe increased. Now whenever you will see that there will be increase then you have to change the variables  $x$  in such way that so that your you know deviation from this left hand side to right hand side will be reduced.

So in that direction you have to go. Like this here shown in this you know slide that if you are considering here, the  $x$  value as 0.1 and accordingly what should be the function  $f(x)$  will come. That will be is equal to it will be expressed as like  $x$  minus exponent of  $-2x$ . That will be equals to zero. This is very simple that it will be  $x$  minus exponent of  $-2x$ .

This is basically the you know deviation of this left hand side to right hand side. Or you can express this as a function of  $x$  minus exponent of  $-2x$  so that your  $x$  value, corresponding  $x$  value will give you that function of this you know  $x$  minus exponent of  $-2x$  will be equals to 0 or very near about to 0.

Now in this case you will see that if you consider this  $x$  is equal to 0.1 you will get this function  $f(x)$  will be equals to - 0.7187305 you know 753 like this. Similarly, if

you increase that value 0.2 its value is coming like this here. This you know it is not coming to exactly 0 as  $f(x)$  is equal to 0, but if you change this value of 0.3 you will see that this you know deviation is coming to reduced here. Here 0.7 to 0.2 it is coming.

Whereas if you keep on increase that value of  $x$  here 0.32 suppose if you assume here 0.426156 you will see that this value of  $f(x)$  will be is equal to you know that is -2.73 into 10 to the power -4. This is you know very near about to zero you can say. So in this case you are getting this  $f(x)$  for this corresponding value of  $x$  here.

If you again increase the value of  $x$  here, here 0.5 you will see that this value is coming to increase again 0.132120556 here. Again if you increase that value 0.6 it will again it will increase to 0.29 and if you keep on increasing this value, you will see there you know function of  $x$  that is  $f(x)$  will you know gradually increased.

So here initially it is decreased and then increased then it will be seen it will come here at 0.426153. It is seen that this you know function's value is coming almost equals to zero. So we can consider here the value of  $x$  will be equals to 0.426156 which will give you that function  $f(x)$  will be near about to zero.

So in this way we can you know find out what will be the solution of this you know nonlinear equation. So this is called spreadsheet solution but it is trial and error. It will take a lot of time to you know find out this you know a solution of this nonlinearly equation.

But you can do by you can use other computational you know programming or you can use that you know computer program by which you can you know solve this easily. Or otherwise you can you know do a graph  $x$  versus  $f(x)$  versus know  $x$ . There you will see that where this minimum value of  $x$  will be coming or what will be the value of  $x$  will be coming where that  $f(x)$  will be minimum.

So in that way you can also find out what should be the solution of this nonlinear equation.

**(Refer Slide Time: 09:40)**

## Newton's (mostly used) method:

- Newton's method is one of the most popular numerical methods.
- This method originates from the Taylor's series expansion of the function  $f(x)$  about the point  $x_1$ :

$$f(x_1) + (x - x_1)f'(x_1) + \frac{1}{2!}(x - x_1)^2 f''(x_1) + \dots \quad (1)$$

where  $f$ , and its first and second order derivatives,  $f'$  and  $f''$  are calculated at  $x_1$ .

Now we will then do that Newton's method to solve this nonlinear equation which is mostly used and this is actually one of the most popular numerical methods and this is basically originates from the Taylor's you know series expansion of the function about the point suppose  $x_1$  initial point.

And in this case, if we write that you know Taylor series here for the expansion of this function  $f(x)$  at this point  $x_1$ , we can write here,  $f(x_1)$  will be plus sorry  $f(x_1) + (x - x_1)$  into  $f'$  of  $f'$  dash  $x_1$  plus  $\frac{1}{2}$  you know factorial into  $(x - x_1)$  whole square into  $f''$  double dash  $x_1$  plus ...

**(Refer Slide Time: 10:42)**

If we take the first two terms of the Taylor's series expansion we have:

$$f(x) \approx f(x_1) + (x - x_1)f'(x_1) \quad (2)$$

We then set Eq. (2) to zero (i.e.  $f(x) = 0$ ) to find the root of the equation which gives us:

$$f(x_1) + (x - x_1)f'(x_1) = 0 \quad (3)$$

Rearranging the Eq. (3) we obtain the next approximation to the root, giving us:

$$x = x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} \quad (4)$$

After that if we take the first two terms of the Taylor's series expansion then we have  $f(x)$  will be equals to  $f(x_1)$  plus  $(x - x_1)$  into  $f'$  dash  $x_1$ . Now we then set equation

two here to 0. That is  $f(x)$  will be equals to 0 to find the root of the equation which gives us like this  $f(x_1) + (x - x_1)$  into  $f'(x_1)$ .

That will be equals to 0 as shown here in the equation number 3. Now if we rearrange this equation number 3 we can get the next approximation to the root given as you know  $x$  will be equals to then  $x_2$ . That will be is equal to  $x_1 - \frac{f(x_1)}{f'(x_1)}$ . So from this basically what we did here, we took that you know two terms of the Taylor series expansion there.

And after that we are considering that  $f(x)$  will be equals to 0 and then from which we can find out what should be the value of  $x$ . So this  $x$  will be basically the initial value of the next step that will be is equal to  $x_2$ . So this  $x_2$  will be is equal to then  $x_1 - \frac{f(x_1)}{f'(x_1)}$ .

So here basically what will be the initial value of this  $x$  and minus then function of that  $x$  at the value of  $x_1$  and also what will be the first derivative of that, you know function at point  $x_1$  that you have to you know take a ratio for that and then you have to subtract this ratio from that initial value of that  $x$ .

**(Refer Slide Time: 12:56)**

Thus generalizing Eq. (4) we obtain Newton's iterative method:

$$x_i = x_{i-1} - \frac{f(x_{i-1})}{f'(x_{i-1})}, i \in \mathbb{N}$$

Since  $x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$

and if  $x_i = x_{i+1}$ , then

$$x_i = x_i - \frac{f(x_i)}{f'(x_i)}$$

This implies that  $\frac{f(x_i)}{f'(x_i)} = 0$

thus  $f(x_i) = 0$

*x<sub>i</sub> is the i<sup>th</sup> estimate of root. Successive estimates are then generated with a test for convergence*

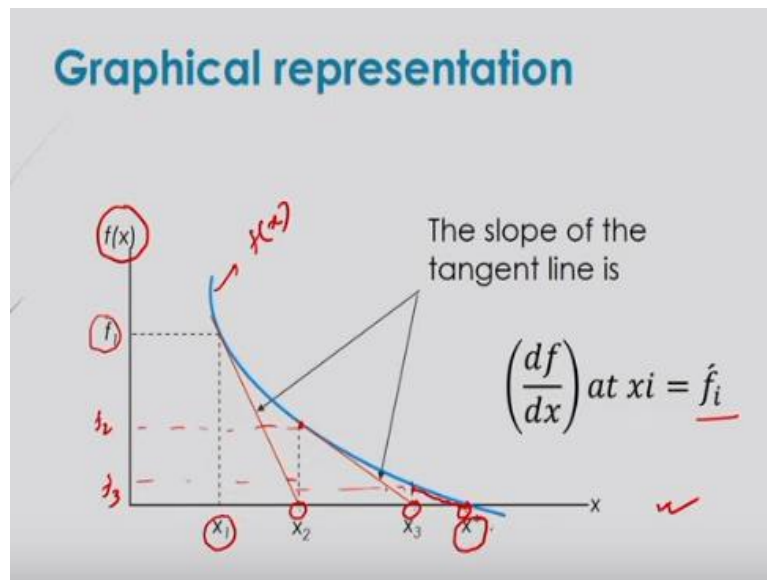
So in this way keep on that assuming that what should be the you know next value of  $x$  just by taking that function at point  $x$  and also ratio of this function to which the first derivative at that particular point. So if we generalize this you know condition of that

finding the successive  $x$  then we can write here  $x_i$  will be equals to  $x_{(i-1)} - f(x_{i-1})$  divided by  $f'(x_{i-1})$ .

Where  $i$  will be you know that 1, 2, 3, 4 like this. And since here  $x_{i+1}$  that will be is equal to  $x_i - f(x_i)$  by  $f'(x_i)$  and if  $x_i$  will be equals to  $x_{i+1}$  then we can write here  $x_i$  will be is equal to  $x_i - f(x_i)$  divided by  $f'(x_i)$ . So this implies that  $f(x_i)$  by  $f'(x_i)$  that will be equals to 0.

What does it mean that at any point  $x$  that function will be equals to 0. So this is the main principles of this you know Newton's method by which you can solve the nonlinear equation. So in this case  $x_i$  is the  $i$ th estimate of the root and successive estimates are then generated with a test of convergence, when that function will come to 0.

**(Refer Slide Time: 14:35)**



Now if we represent it graphically, we can then have this you know diagram or figure here like this, the y axis we can, you know consider  $f(x)$  and in x axis that is  $x$  successive value of you know  $x$  here. If you consider that initial point of that  $x$  then  $x_1$  then this is your function simply  $f(x)$ .

So at this function profile at point  $x_1$  what should be the function value it is  $f_1$ . Similarly, at this point  $x_1$  if you make a tangent at this point you will see that tangent will you know intersect this x axis at point  $x_2$ . Now at this point  $x_2$  if you go to that



profile here  $f(x)$  then corresponding  $f'(x)$  will be is equal to here like this. So this will be your  $f''(x)$ .

Similarly, again at this point  $x_2$  at this, you know on this, you know profile if you make again the tangent of this profile then this tangent will you know intersect the  $x$  axis at point  $x_3$ .

Now at this  $x_3$  point again you will see that if you consider what should be the value of function here and if it is represented by  $f_3$  then we can consider here at this point  $f_3$  again if you make a tangent, you will see there will be a you know intersection at  $x$  axis  $x$  at  $x^*$  and this at this point of  $x^*$  you will see that this  $f(x)$  will be coming almost equals to 0. That means here  $x^*$ ,  $f(x)^*$  will be equals to 0.

So in this way you will see that at different point of  $x$  whenever you are making any slope or tangent and when it intersects to that  $x$  axis that will be your next you know successive point of  $x$  and at when this you know functions will be coming zero at that particular successive points that will give you the root or solution of that nonlinear equation.

So here we can write that  $df$  by  $dx$  that means  $x$  dash at  $x_i$  that will be is equal to  $f_i$  dash that  $f_i$  dash here we will see that, when it will intersect that  $x$  axis and at that particular point, if this function  $x$  function  $f(x)$  will comes to zero, then you will get that final root of that nonlinear equation.

**(Refer Slide Time: 17:45)**

First Iteration	$x_1 = 0.2$ $\Downarrow$ $f'(x_1) = 1 + e^{-0.2} = 1.8187$ $\Downarrow$ $x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 0.5402$	Third Iteration	$x_3 = 0.5670$ $\Downarrow$ $f(x_3) = 0.5670 - e^{-0.5670} = 2.246 \times 10^{-1}$ $\Downarrow$ $f'(x_3) = 1 + e^{-0.5670} = 1.5672$ $x_4 = x_3 - \frac{f(x_3)}{f'(x_3)} = 0.56714$
Second Iteration	$x_2 = 0.5402$ $\Downarrow$ $f(x_2) = 0.5402 - e^{-0.5402} = -0.0424$ $\Downarrow$ $f'(x_2) = 1 + e^{-0.5402} = 1.5826$ $x_3 = x_2 - \frac{f(x_2)}{f'(x_2)} = 0.5670$	<p><b>At the value of <math>x_4 = 0.56714</math> the function <math>f(x)</math> is very nearly equal to zero (<math>= -5.15655 \times 10^{-06}</math>)</b></p>	

Let us do an example here for this. Now you have to determine the root of the equation here. Suppose  $x$  is equal to  $e$  to the power  $-x$  using this Newton's method. Now  $f(x)$  will be equal to basically  $x$  minus  $e$  to the power  $-x$ . This is your  $f(x)$ . Now what should be the derivative of this first derivative of this function.

It will be equal to a  $f'$  dash  $x$ , that will be equal to  $df$  by  $dx$ . This is basically  $1$  plus  $e$  to the power  $-x$  as shown here in the slide. Now when  $x$  is equal to zero,  $f(x)$  is in negative, whereas when  $x$  is equal to  $1$ ,  $f(x)$  is coming positive, therefore, we can say that the root  $x^*$  must be between  $0$  and  $1$ .

So in this case, if we assume that the initial value of  $x$  as  $x_1$  is equal to  $0.2$ , then first iteration by this  $x_1$  is equal to  $0.2$ . We can write then  $f'$  dash  $x_1$  that means first derivative of that function at this point  $x_1$  is equal to  $0.2$ . It will come  $1$  plus  $e$  to the power  $-0.2$ . That means here  $1.8187$ . So what should be the successive point of this  $x_1$ ?

It will be coming  $x_2$ . This  $x_2$  will be becoming as per this Newton's method. It will be  $x_1$  minus  $f(x_1)$  divided by  $f'$  dash  $x_1$ . What is the  $x_1$  value? It is given  $0.2$  and  $f(x_1)$  that is basically what is that after substitution of  $x_1$  in that function you know  $x$  it will be coming as whatever value and then divide it by this  $f'$  dash  $x$  then it will be becoming us finally  $0.5402$ .

Now this  $x_2$  value of 0.5402 it will be your first or initial guess of that second iteration. So in the second iteration the initial value is  $x_2$ . That will be is equal to 0.5402. And then  $f(x_2)$  will be is equal to what 0.5402 minus  $e$  to the power -0.5402. Then it will be coming as -0.0424 and then what should be the first derivative of that function at this  $x_2$  value?

It will be  $1 + e$  to the power -0.5402. Then it will come 1.5826. Now with this values of  $f(x_2)$ ,  $f'(x_2)$  and initial value of  $x_2$ , we can calculate the successive value of  $x_3$  which will be the initial value of the third iteration. So this  $x_3$  will be equals to  $x_2 - \frac{f(x_2)}{f'(x_2)}$ . This is basically based on the principle of Newton's method.

Then after substitution of this value, we can get this value of  $x_3$  as 0.5670. Now see the third iteration, this  $x_3$  will be equals to your first guess of that  $x$  value. So  $x_3$  is equal to 0.5670 its initial value of this third iteration, and then find what will be the  $f(x_3)$  that will be coming as  $2.246 \times 10^{-4}$ .

And then first derivative of this function at this  $x_3$  point it will be as  $1 + e$  to the power minus 0.5670. It is coming 1.5672. After that to find out the next point of  $x$  that means  $x_4$  here, it will be as per principle of Newton's law, it will be  $x_3 - \frac{f(x_3)}{f'(x_3)}$ . After substitution of this value of  $x_3$ ,  $f(x_3)$  and  $f'(x_3)$  it will come 0.56714.

Now see, at this value of  $x_4$ , you will see that 0.56714, the function  $f(x)$  is very nearly equals to 0. This will give you the value as  $-5.15655 \times 10^{-6}$ . So it is very near about to 0. So that is why we can say we can stop the iteration here and we can consider that solution of this equation will be equals to here 0.56714.

So in this way you can solve the nonlinear equation by trial and error method as per this you know Newton's method. Now let us now consider the solving a set of nonlinear algebraic equations involving multiple variables.

**(Refer Slide Time: 23:10)**

## Solving a set of nonlinear algebraic equations involving multiple variables

- In the previous example we solved the equation for single variable and single equation
- The same Newton's method can be used for multivariate and multiple equations by modifying the Newton's method

So till now we have described how to solve single nonlinear equation by Newton's method. Now in this case we will describe how to solve the nonlinear algebraic equations, there will be a set of nonlinear algebraic equations. There multiple variables will be there. So in the, we can also use here the same Newton's method that will be used for that multiple equations by modifying this Newton's method.

**(Refer Slide Time: 23:52)**

- In this case, the nonlinear system is to be expressed as a matrix with a corresponding vector as:

$$\underline{x^{(k)}} = \underline{x^{(k-1)}} - \underline{J(x^{(k-1)})^{-1}} \underline{F(x^{(k-1)})}$$

- where  $k = 1; 2; \dots; n$  represents the iteration
- $\mathbf{F}$  is a vector function, and  $J(\mathbf{x})^{-1}$  is the inverse of the Jacobian matrix .
- This equation represents the procedure of Newton's method for solving nonlinear algebraic systems. ♦

And in this case, you have to consider some other you know some matrix, it will be called as Jacobian matrix for this modification of this Newton's method. So in this case, the nonlinear system is to be expressed as a matrix with that corresponding vector as  $x_k$  that will be is equal to  $x_{k-1}$  minus Jacobian matrix at that  $k-1$  that value of  $x$  to the power -1 into function of that  $k-1$  th value of that variable  $x$ .

So in this case  $k$  will be equals to 1, 2,  $n$  which will represent the iteration. Now so we can say that  $x^k$  will be equals to  $x^{k-1} - J^{-1} f(x)$  to the power  $k-1$ . So this is your iteration procedure based on which you have to find out the solution. Now this  $f$  is a vector function and  $J^{-1}$  is the inverse of the Jacobian matrix.

This equation represents the procedure of Newton's method for solving nonlinear algebraic equation.

**(Refer Slide Time: 25:16)**

■ However, instead of solving the equation  $f(x) = 0$ , we are now solving the system  $\mathbf{F}(\mathbf{x}) = 0$ . We will now go through the equation and define each component.

■ (1) Let  $\mathbf{F}$  be a function

$$\mathbf{F}(x_1, x_2, \dots, x_n) = \begin{bmatrix} f_1(x_1, x_2, \dots, x_n) \\ f_2(x_1, x_2, \dots, x_n) \\ \dots \\ f_n(x_1, x_2, \dots, x_n) \end{bmatrix}$$

$\mathbf{x}$  represents the vector as:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix}$$

Now let us see what should be the function and also Jacobian matrix. Now instead of solving the equation  $f(x)$  is equal to 0 whatever we have described earlier, we are now solving the system of  $f(x)$  equals to 0. In this case, there will be a set of nonlinear equation instead of single nonlinear equation.

So we will now go through the equation and define each component like here, let  $F$  be a function of this here  $f(x_1, x_2, \dots, x_n)$  and this you know function will be a set of nonlinear equation like  $f_1, f_2$  and up to  $f_n$  where  $x$  here represents the vector as a set of this  $x_1, x_2$  up to  $x_n$ .

**(Refer Slide Time: 26:14)**

J(x) is the Jacobian matrix

$$J(x)^{-1} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}(x) & \frac{\partial f_1}{\partial x_2}(x) & \dots & \frac{\partial f_1}{\partial x_n}(x) \\ \frac{\partial f_2}{\partial x_1}(x) & \frac{\partial f_2}{\partial x_2}(x) & \dots & \frac{\partial f_2}{\partial x_n}(x) \\ \dots & \dots & \dots & \dots \\ \frac{\partial f_n}{\partial x_1}(x) & \frac{\partial f_n}{\partial x_2}(x) & \dots & \frac{\partial f_n}{\partial x_n}(x) \end{bmatrix}^{-1}$$

And J x is the Jacobian matrix, which is defined as here, you know first here that means first derivative of you know that function that is by which that set of that function is formed. So it will be doh f 1 doh x 1 into x into doh f 1 by doh x 2 into x up to doh f 1 doh x n into x. Here X capital X is basically set of you know x where x 1 up to x n.

And similarly, here in the second way it will come doh f 2 doh x 1 into x, doh f 2 doh x 2 into x, doh f 2 doh x n into x. If there are n number of equations, then you have to make the derivative of that doh here f (n) into doh x n doh x 1 to x into doh f n doh x 2 into x up to you know that doh f n doh x n into x.

So and this is called Jacobian matrix and inverse of this it will be regarded as inverse of Jacobian matrix.

**(Refer Slide Time: 27:32)**

## Steps of Newton's method

Step 1:

Let  $x^{(0)} = (x_1^{(0)}, x_2^{(0)}, x_3^{(0)}, \dots, x_n^{(0)})$  be a given initial vector. ✓

Step 2:

Calculate  $J(x^{(0)})$  and  $F(x^{(0)})$ .

Step 3:

We now have to calculate the vector  $y^{(0)}$ , where

$$y^{(0)} = -J(x^{(0)})^{-1}F(x^{(0)})$$

You can replace  $-J(x^{(0)})^{-1}F(x^{(0)})$  formula with  $y^{(0)}$ , then

$$x^{(k)} = x^{(k-1)} - J(x^{(k-1)})^{-1}F(x^{(k-1)}) = x^{(k-1)} - y^{(k-1)}$$

Now if we consider that steps of Newton's method based on this, you know nonlinear set equation, then we can say that as a first step what you have to do that, here let  $x_0$  that will be equals to  $x_1 0, x_2 0, x_3 0$ , up to  $x_n 0$ . And it will be the initial vector of those variables  $x_1$  to  $x_n$ .

And the next step what you have to do you have to calculate the Jacobian matrix at that  $x_0$ , that is initial of value, initial guess there, and also what will be the  $f(x)$ . And then after that as a step 3, we have to calculate the vector  $y_0$  where  $y_0$  will be defined as minus of Jacobian matrix at  $x_0$  to the power -1 that means inverse of that Jacobian matrix at that  $x_0$  into function  $x_0$ .

So you can replace this  $-J x_0$  to the power -1 one into  $f(x_0)$  formula with the  $y_0$  here. Then  $x_k$  will be is equal to  $x_{k-1}$  minus  $J x_{(k-1)}$  to the power -1  $f(x)_{k-1}$  it will be equals to  $x_{k-1}$  minus  $y_{k-1}$ . So this step 3. In this way you have to calculate.

**(Refer Slide Time: 29:12)**

**Step 4:**  
 Once  $y^{(0)}$  is found, we can now proceed to finish the first iteration by solving for  $x^{(1)}$ . Thus using the result from Step 3, we have that

$$\underline{x^{(1)}} = \underline{x^{(0)}} + \underline{y^{(0)}} = \begin{bmatrix} x_1^{(0)} \\ x_2^{(0)} \\ \dots \\ x_n^{(0)} \end{bmatrix} + \begin{bmatrix} y_1^{(0)} \\ y_2^{(0)} \\ \dots \\ y_n^{(0)} \end{bmatrix}$$

**Step 5:**  
 Once we have calculated  $x^{(1)}$ , we have to repeat the process again, until  $x^{(k)}$  converges to  $x$ . This indicates we have reached the solution to  $\mathbf{F}(\mathbf{x}) = 0$ , where  $x$  is the solution to the system.

When a set of vectors converges, the norm  $\|x^{(k)} - x^{(k-1)}\| = 0$

$$\|x^{(k)} - x^{(k-1)}\| = \sqrt{(x_1^{(k)} - x_1^{(k-1)})^2 + \dots + (x_n^{(k)} - x_n^{(k-1)})^2} = 0$$

And then in step 4, once  $y_0$  is found, we can now proceed to finish the first iteration, by solving for  $x_1$  thus using the result from the step 3, then we can get  $x_1$  will be equals to  $x_0 + y_0$ . This  $x_0$  will be equals to  $x_1^0, x_2^0$  up to  $x_n^0$  plus  $y_1^0, y_2^0$  up to  $y_n^0$ , these two matrix.

And then once we have calculated this  $x_1$  based on this  $x_0$  and  $y_0$  we have to repeat the process again until  $x_k$  converges to  $x$ . And this indicates we have reached the solution to  $f(x)$  is equal to 0 where  $x$  is the solution to the system. Now when a set of vectors converges, the norm is like this  $x_k$  minus  $x_{(k-1)}$ .

Mod of this will be equals to 0, and then it will be defined as this here root over  $x_1^k$  minus  $x_1^{(k-1)}$  whole square plus  $x_2^k$  minus  $x_2^{(k-1)}$  whole square plus up to like this  $x_n^k$  minus  $x_n^{(k-1)}$  whole square and that will give you equals to 0.

So in this way we can calculate what should be the or we can get what should be the root of that or solution of that set of nonlinear equation just by converging to  $x$ , the value of whatever guess we are considering as a step by step and successive value of  $x$  as per that Newton's method will give you that convergence of that  $x$  and which will be considering as the solution of the set of you know nonlinear equation.

Now advantages and disadvantages of this Newton's method to solve this, you know nonlinear equation like this.

**(Refer Slide Time: 31:36)**



## Advantages and Disadvantages of Newton's Method

- Advantages of Newton's method: Its not too complicated in form and it can be used to solve a variety of problems.
- The major disadvantage: is that  $J(x)$ , as well as its inversion has, to be calculated for each iteration.
- Calculating both the Jacobian matrix and its inverse can be quite time consuming depending on the size of your system.
- Another problem is that it may fail to converge.
- If Newton's method fails to converge this will result in an oscillation between points

Advantages of Newton's method is that it is not too complicated in form and it can be used to solve a variety of, you know problems. The major disadvantage is that, this here Jacobian matrix as well as its inversion has to be calculated for each iteration. So it will take you know a long time to finish and also calculating both the Jacobian matrix and its inverse can be quite time consuming that depending on the size of your system.

Another problem is that it may fail to converge. If Newton's method fails to converge this will result in an oscillation between points there. So there will be a issue for that. So otherwise, it is advantageous because it will not be too complicated system to solve the equation.

**(Refer Slide Time: 32:39)**

### Example

$$3x_1 - \cos(x_2 x_3) - 0.5 = 0$$

$$x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06 = 0$$

$$e^{-x_1 x_2} + 20x_3 + \frac{10\pi - 3}{3} = 0$$

Consider the initial approximation is

$$x^{(0)} = \begin{bmatrix} 0.1 \\ 0.1 \\ -0.1 \end{bmatrix}$$

Now let us do an example based on this you know Newton's method for a set of nonlinear equation to solve. Here is example given in the slides here. Here one equation is like this  $3x_1 - \cos(x_2x_3) - 0.5$  that will be equals to 0. Here one equation, this is nonlinear equation.

Another equation is given  $x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06$  is equals to 0. And then third equation is given  $e^{-x_2x_3} + 20x_3 + \frac{10\pi - 3}{3}$  That will be equals to zero. This is another equation. So here three you know nonlinear equation given to you and you have to find out the, you know solution of this  $x_1, x_2$  and  $x_3$ .

Now consider the initial approximation is here  $x_0$  is 0.1, 0.1 and - 0.1. So based on this, you have to solve this nonlinear equation to find out the solution for  $x_1, x_2$  and  $x_3$ .

**(Refer Slide Time: 34:06)**

**Solution**

- Step 1: We have our initial vector
 
$$x^{(0)} = \begin{bmatrix} 0.1 \\ 0.1 \\ -0.1 \end{bmatrix}$$
- Step 2: Define  $F(x)$  and  $J(x)$ :
 
$$F(x) = \begin{bmatrix} 3x_1 - \cos(x_2x_3) - 0.5 \\ x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 + 1.06 \\ e^{-x_2x_3} + 20x_3 + \frac{10\pi - 3}{3} \end{bmatrix}$$

$$J(x) = \begin{bmatrix} 3 & x_3 \sin(x_2x_3) & x_2 \sin(x_2x_3) \\ 2x_1 & -162(x_2 + 0.1) & \cos x_3 \\ -x_2e^{-x_2x_3} & -x_1e^{-x_2x_3} & 20 \end{bmatrix}$$

Now first of all, that you have to follow that step 1, what should be the initial, you know vector. Since it is given that you have to assume this initial vector as  $x_0$  is equal to 0.1, 0.1 and - 0.1. This is basically  $x_1$  is equal to 0.1  $x_2$  is equal to 0.1 and  $x_3$  is equal to - 0.1 at its initial guess. Then, step 2 you have to define  $F(x)$  and  $J(x)$ .

That means function set of you know function and also Jacobian matrix. So  $F(x)$  is here, simply this is  $3x_1 - \cos x_1, x_2$  into  $x_3 - 0.5$  here. And then here  $x_1$

square minus  $81 \times 2 + 0.1$  square plus  $\sin x^3 + 1.06$ . And then third equation here given. So these actually made this you know function  $F(x)$ .

And then Jacobian matrix simply the derivative of this you know function  $F(x)$  based on that variables there. So it will be coming as  $3 \times 3$   $\sin x^2 \times 3$ ,  $x^2 \sin x^2 \times 3$  here. And then what is that  $2 \times 1$  minus you know  $162$  into  $x^2 + 0.1 \cos x^3$  and then  $-x^2 e$  to the power minus  $x^1 \times 2$  and then minus  $x^1 e$  to the power  $-x^1 \times 2$  and then  $20$  like this.

So in this way, you can find out what should be the Jacobian matrix for that initial value.

**(Refer Slide Time: 36:08)**

Calculate

$F(x^{(0)})$  and  $J(x^{(0)})$

Where

$$F(x^{(0)}) = \begin{bmatrix} 0.3 - \cos(-0.01) - 0.5 \\ 0.01 - 3.24 + \sin(-0.1) + 1.06 \\ e^{(-0.01)} + 2 + \frac{10\pi - 3}{3} \end{bmatrix} \begin{bmatrix} -1.1995 \\ -2.269833417 \\ 8.462025346 \end{bmatrix}$$

$$x^{(0)} = (0.1, 0.1, -0.1)^T$$

$$J(x) = \begin{bmatrix} 3 & (-0.1)\sin(-0.01) & 0.1\sin(-0.01) \\ 0.2 & -32.4 & \cos(-0.1) \\ -0.1e^{-0.01} & -0.1e^{-0.01} & 20 \end{bmatrix}$$

$$= \begin{bmatrix} 3 & 0.000999983 & -0.000999983 \\ 0.2 & -32.4 & 0.995004165 \\ -0.099004984 & -0.099004983 & 20 \end{bmatrix}$$

Now for this initial value of this function,  $F(x^0)$  and Jacobian matrix zero will be equals to here, after substitution of value of  $x^0$  here in the  $F(x)$  it will be coming as like this, and then here Jacobian matrix here, it will be like this as a transport here. So it will be coming as this after substitution of this value, this will be your Jacobian matrix.

**(Refer Slide Time: 36:38)**

Step 3: Solve the system

$$\underline{J(x^{(0)})y^{(0)} = -F(x^{(0)})}$$

using Gaussian Elimination:

$$\begin{bmatrix} 3 & 0.000999983 & -0.000999983 \\ 0.2 & -32.4 & 0.995004165 \\ -0.099004984 & -0.099004983 & 20 \end{bmatrix} \begin{bmatrix} y_1^{(0)} \\ y_2^{(0)} \\ y_3^{(0)} \end{bmatrix} = - \begin{bmatrix} -1.19995 \\ -2.2698333417 \\ 8.462025346 \end{bmatrix}$$

After solving

$$y^{(0)} = \begin{bmatrix} 0.40003702 \\ -0.08053314 \\ -0.42152047 \end{bmatrix}$$

And then, to solve this you have to consider that Jacobian matrix  $x_0$  into  $y_0$ . That will be is equal to minus  $F(x_0)$ . Now then, using Gaussian elimination method, we can have this to solve after that finally we can get this here for this  $y_1_0$ ,  $y_2_0$  and  $y_3_0$  here. Then we can get here  $y_0$  as will be equals to here as per this matrix it will be coming as 0.4003702 and -0.08053314.

And then  $y_3$  will be equals to -0.4215047. So here this will be your, you know  $y_0$  as per that Newton's method whatever we have described earlier.

**(Refer Slide Time: 37:34)**

Step 4: Using the result in Step 3, compute

$$x^{(1)} = x^{(0)} + y^{(0)}$$

$$x^{(1)} = \begin{bmatrix} 0.1 \\ 0.1 \\ -0.1 \end{bmatrix} + \begin{bmatrix} 0.40003702 \\ -0.008053314 \\ -0.42152047 \end{bmatrix}$$

$$= \begin{bmatrix} 0.50003702 \\ 0.01946686 \\ -0.52152047 \end{bmatrix}$$

**We can use the results of  $x^{(1)}$  to find our next iteration  $x^{(2)}$  by using the same procedure.**

And then next guess of you know initial value of  $x$  that will be equals to  $x_1$ , this is basically  $x_0 + y_0$ , then it will be coming as your as per that matrix rule that will be equals to here 0.50, 0.0194 and -0.5215. So this will give you what is that  $x_1$  value.

Again then you have to use this  $x_1$  value to find out what will be the  $F(x)$  at that  $x_1$  and Jacobian matrix at that you know  $x_1$  value. So we can use this results of  $x_1$  to find our next iteration  $x_2$  by using the same procedure.

**(Refer Slide Time: 38:22)**

Step 5:  
If we continue to repeat the process, we will get the following results:

$k$	$x_1^{(k)}$	$x_2^{(k)}$	$x_3^{(k)}$	$\ x^{(k)} - x^{(k-1)}\ $
0	0.10000000	0.10000000	-0.10000000	-
1	0.50003702	0.01946686	-0.52152047	0.422
2	0.50004593	0.00158859	-0.52355711	0.0179
3	0.50000034	0.00001244	-0.52359845	0.00158
4	0.50000000	0.00000000	-0.52359877	0.0000124
5	0.50000000	0.00000000	-0.52359877	0

$\bar{x} = \begin{bmatrix} 0.50000000 \\ 0.00000000 \\ -0.52359877 \end{bmatrix}$  is an appx. solution

F(x) has converged to the solution

So if we continue to repeat this procedure, we will get the following results here for you know  $k$  here 0, 1, 2, 3, 4 that means here iteration number. Here for this first iteration it is you know it is given here and then second iteration we have found that this value and then the third iteration here, what will happen?

After that  $x_1$  plus you know  $y_0$  it will be coming like this and then keep on continuing the repetition of the process based on that, you know Newton's method we can have at different  $k$  value we can get different value of  $x_1$ ,  $x_2$  and  $x_3$ . And then you will see that at this fifth iteration of this you will see that the value of  $x_1$  will be coming as 0.5 and  $x_2$  will be equals to almost 0 and  $x_3$  will be equals to -0.5235987.

And finally, you will see that this deviation  $x_k - x_{k-1}$  will be equals to 0 where you have to stop the iteration. So parallel you have to find out what should be the you know deviation of this  $x_k - x_{k-1}$ . And if it is coming almost equals to 0 then you have to stop your iteration.

And that you know iteration will give you the corresponding value of  $x_1$ ,  $x_2$  and  $x_3$  and those value will be you know treated as the solution of that set of nonlinear

equation. So here  $x$  will be at that point it will be equals to 0.50 and -0.52359877. So this is an approximate solution of those you know nonlinear equation.

Here we have 3 nonlinear equation 3 unknown variables and those 3 unknown variables are 0.5, 0, and 0.523 like this. So in this way you can you know calculate or you can estimate the solution of nonlinear equation and this is the best way to find out the you know solution of nonlinear equation if there are more than one nonlinear equation.

Even you can use that, you know single equation to find out that solution for its nonlinearity based on that, you know Newton's method. So we have given here two examples and two you know procedure of that Newton's method. One is simple Newton's method just by guessing this initial value and successive value will be coming based on the, you know function value, and its first derivative.

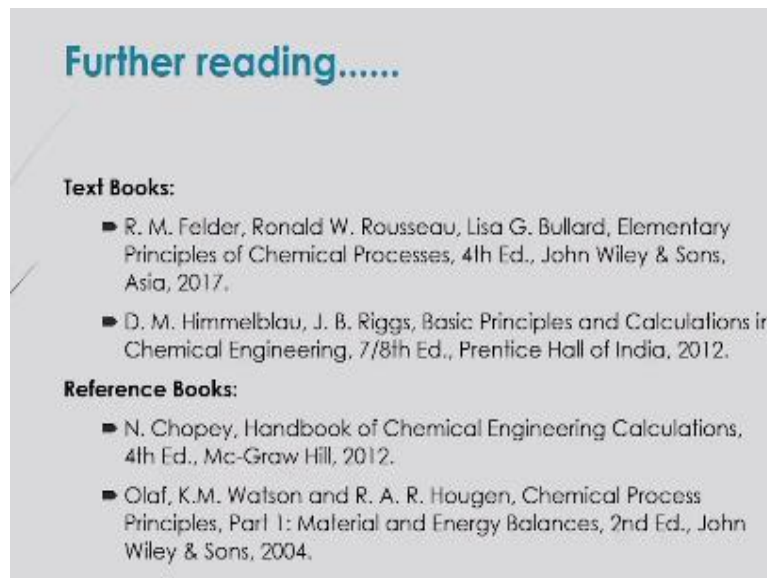
And then what should be the second guess that according to that, you know principle of that, you know subtracting that ratio of that function value to the you know first derivative from the initial guess then you will get the second guess. So in this way, keep on you know repeating that you know that solution of that equation until this function will come to 0 that will give you the solution of single nonlinear equation.

But for the set of you know nonlinear equation to find the solution here, in this case, you have to you know modify that Newton's method just by you know incorporating the that is Jacobian matrix. And from that Jacobian matrix you have to you know calculate the next guess of that or next iteration of that  $x$  value just incorporating that, you know Jacobian matrix with those you know function value.

And you have to you know continue this iteration in this method until there is a deviation of this you know initial guess to the final or previous that means, successive guess, it will be if that deviation is coming 0 for those you know values of you know  $x_k$  minus  $x_{(k-1)}$  then you have to stop there that iteration and respective value of  $x_1$ ,  $x_2$ , and  $x_3$  will give you the solution of that set of nonlinear equation.

So I think it will be helpful to solve any nonlinear equation based on this method.

(Refer Slide Time: 43:14)



**Further reading.....**

**Text Books:**

- ▶ R. M. Felder, Ronald W. Rousseau, Lisa G. Bullard, Elementary Principles of Chemical Processes, 4th Ed., John Wiley & Sons, Asia, 2017.
- ▶ D. M. Himmelblau, J. B. Riggs, Basic Principles and Calculations in Chemical Engineering, 7/8th Ed., Prentice Hall of India, 2012.

**Reference Books:**

- ▶ N. Chopey, Handbook of Chemical Engineering Calculations, 4th Ed., Mc-Graw Hill, 2012.
- ▶ Olaf, K.M. Watson and R. A. R. Hougen, Chemical Process Principles, Part 1: Material and Energy Balances, 2nd Ed., John Wiley & Sons, 2004.

So I would further request you, you know follow some you know example of this Newton's method to solve the nonlinear equation there. And next lecture we will discuss more about that computation techniques. There we will discuss about the numerical integration, how to integrate the you know scattered data based on some principles that will be discussed. So thank you for your attention.