Computational Science in Engineering
Prof. Ashoke De
Department of Aerospace Engineering
Indian Institute of Technology - Kanpur

Lecture - 27
Numerical Analysis

So, now we have just looked at whatever the for a particular numerical method, how you can express or approximate the function through Taylor series and what are the other issues related to error, stability and how the error should be minimised? Now, with that, we are going to look at in details, now, first thing that we are going to talk about the root of the equations or the polynomial equations.

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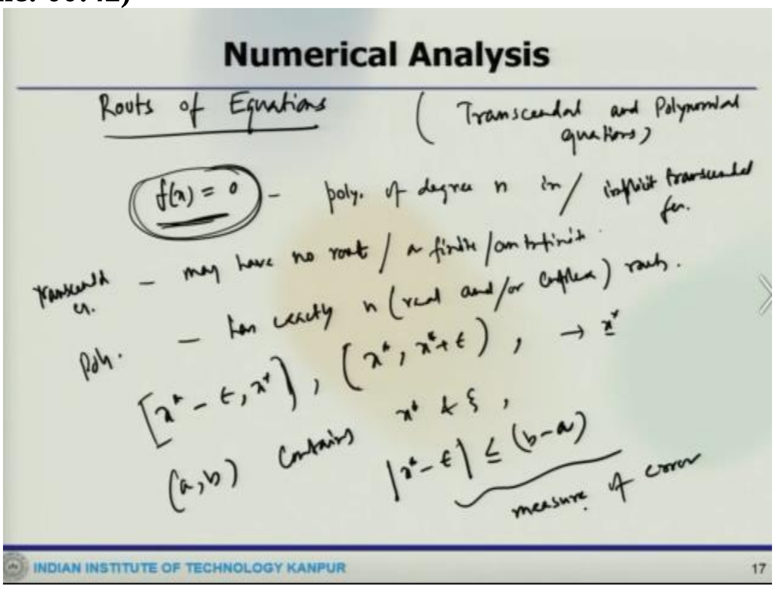

So, that is how we start with that and here we will talk about different methods and how one can find out roots of equation. So, essentially this talk about your some sort of an it could be like, transcendental and or, or rather and polynomial equations. So, that is what we are going to look at it so, how do we find out root and all these things. Now, here we consider the methods for determining the root of an equations were $f(x) = 0$, which may be given explicitly as a polynomial of degree.

So, this is a polynomial of degree n in x or effects may be defined implicitly as a transcendental function implicit transcendental function. Now, a transcendental equation which is given in this particular form may have no root or finite or an infinite number of real and complex roots while a polynomial equation like this, so, this is true for transcendental equation. Now, the polynomial equation of that form has exactly n real and or, or complex roots.

Now, if the function a fixed changes sign in any one of the intervals like $[x^* - \epsilon, x^*]$ or like $[x^*, x^* + \epsilon]$ then x^* defines an approximation to the root of $f(x)$ with accuracy epsilon. Now, this is known as intermediate value theorem hence if an interval us say we define a and b which contains x^* and ξ, where ξ is the exact root of this particular equation which is sufficiently small then we can write that $|x^* - \epsilon| \leq (b - a)$. So, this can be used as a measure of error so, this is the measure of error.

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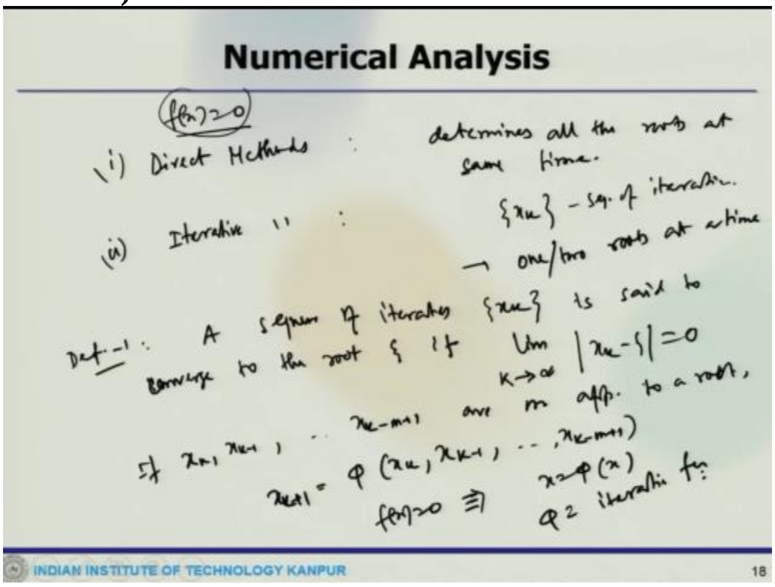

So, there are two different types or the types of methods that can be used to find the root of the equation. So, the function has like this that there are two methods either one can have direct methods. Now, this method gives the exact value of the roots in the absence of roundoff error in a finite number of steps and these methods determine all the roots at the same time and here the error is zero or it could be either the iterative method.

So, these methods or the any iterative methods, they are based on the idea of successive approximation. So, it can start with one or more initial approximation to the root then we will obtain a sequence of iterations like x_K. So, that could be the sequence of iterations which is limit converges to the root. So, here one can find out 1 or 2 roots at a time, but the process may have some errors which are associated with that.

So, now one can have some definition like a sequence of iterates like x_K is said to converge to the root ξ if limit

$$\lim_{K \to \infty} |x_K - \xi| = 0$$

Now, if

$$x_K, x_{K-1}, \dots, x_{K-m+1}$$

are m approximate to a root then we write an iteration method in the form like

$$x_{K+1} = \phi(x_K, x_{K-1}, \dots, x_{K-m+1})$$

where we have written that we can write this particular equation in the equivalent form. So, the $f(x) = 0$, equivalency one can write like $x = \phi(x)$ and the ϕ is called the iteration function.

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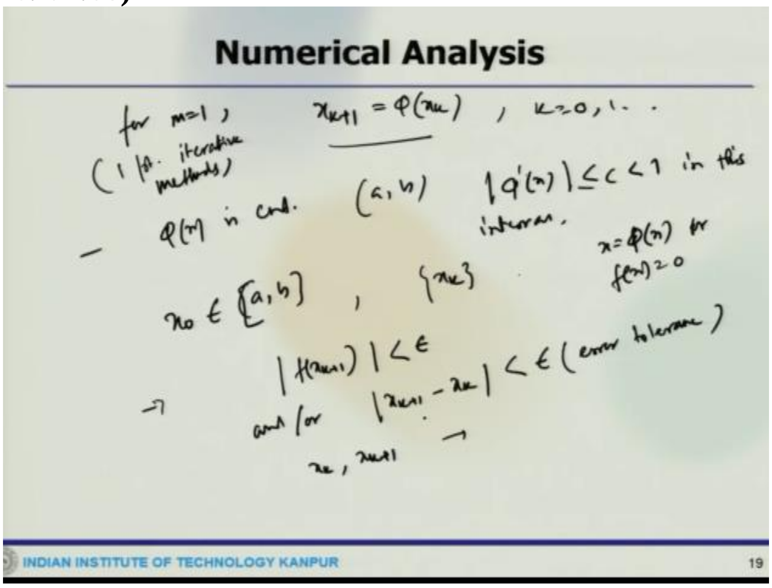

So, for example, for m = 1 we get 1 point iteration method which is called

$$x_{K+1} = \phi(x_K)$$

K = 0, 1, 2 so, this is one point iterative methods. Now, secondly, if $\phi(x)$ is continuous in the interval a and b that contains the root and $|\phi'(x)| \leq C < 1$ in this interval then for any choice of x_0 which is x_0 belongs to a and b any choice of x_0 the sequence of iterates that is x_k obtained from this particular expression converges to the root of $x = \phi(x)$ or $f(x) = 0$.

So, one can say that for any iterative method of the form which is written either like in this particular form or it is written in this particular form. So, we need the iteration function $\phi(x)$ one or more initial approximation to the root. So, in practically expression or application it is not always possible to find ξ exactly. So, we therefore, attempt to approximate the x_{K+1} in such a way that $f(x_{K+1})$ less than epsilon and or $|x_{K+1} - x_K|$ which is less than epsilon where x_K and x_{K+1} are 2 consecutive iterates and epsilon is the prescribed error tolerance. So, this is error tolerance and these are the successive iteration.

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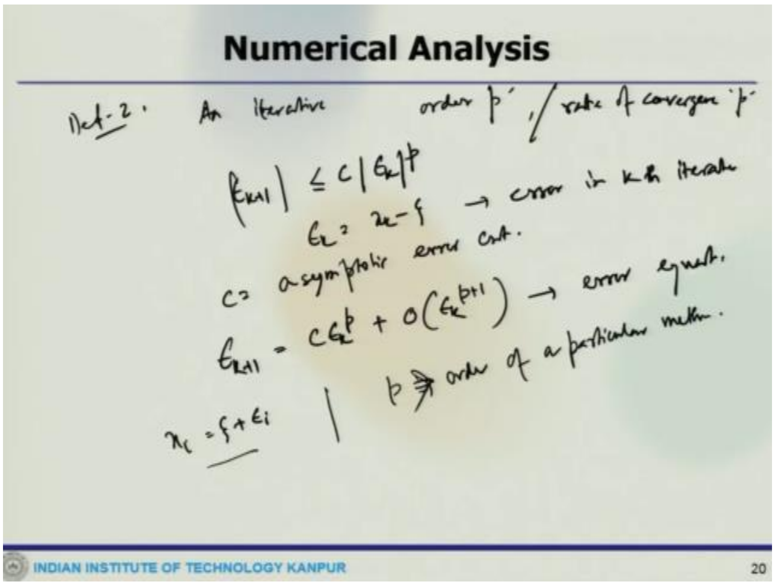

Now, second definition what we can say that an iterative method is said to be of order p or has the rate of convergence p if p is the largest possible real number for which we can write

$$|\epsilon_{K+1}| \leq C|\epsilon_K|p$$

So,

$$\epsilon_K = x_K - \xi$$

It is the error in Kth iterate. So, this is the error in the K th iterate. So, the constant C is called asymptotic error constant. So, it depends on various order derivatives of effects evaluated at ξ and is independent of K.

So, the relation which we can write

$$\epsilon_{K+1} = C\epsilon_K p + O(\epsilon_K{}^{p+1})$$

which is called the short run error equation now, we can substitute

$$x_i = \xi + \epsilon_i$$

for all i in any iteration method and simplifying we obtain the error equation for that method. So, value of p therefore, can be obtained and this is called the order of that method. So, the p is going to tell us the order of a particular method. So, that is what it is going to look at now, how are we going to do that?

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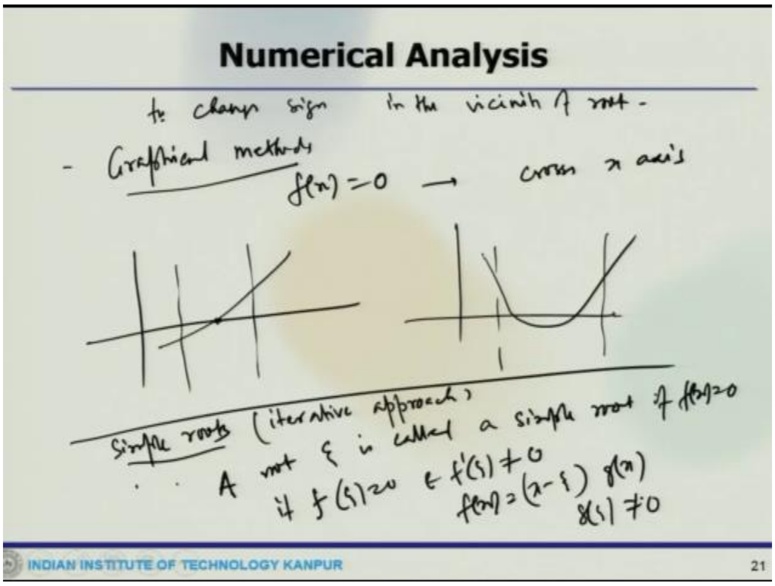

So, the simple approach that now if we say the function which is changing sign in the vicinity of a root then we can use some sort of and so, these are simple approach and we can call as a so, that means the function changes sign in the vicinity of root. So, we can say these are called bracketing methods and all this. So, one of such popular one is to look at is that like graphical methods.

So, the graphical methods what you can have been that this is a simple method for obtaining an estimate of the root of the $f(x)$ equation or the function which is given as $f(x) = 0$ and where we can make a plot of the function and observe that where it crosses x axis. So, this point which represents the value of the $f(x) = 0$ provide the approximation of the root. So, like one can see graphically that this is a function where there is some bound then this could be so, this is where that change the sign.

And this is one of the roots then the function could be like this where this is again an approximate. So, these are representing the graphical way one can find out that. So, the other option is that, but these are not very popular because this is not going to be that easy way to look at the roots and something like that. So, the alternative way that one can look at the iterative approach for these simple roots, these simple roots using iterative approach.

So, one of such approach is that called the bisection method. Now in an iterative approach, what do we say that rather before we can say that a root ξ is called a simple root of $f(x) = 0$, if $f(\xi) = 0$ and $f'(\xi) \neq 0$, then we can also write

$$f(x) = (x - \xi)g(x)$$

where $g(x) \neq 0$.

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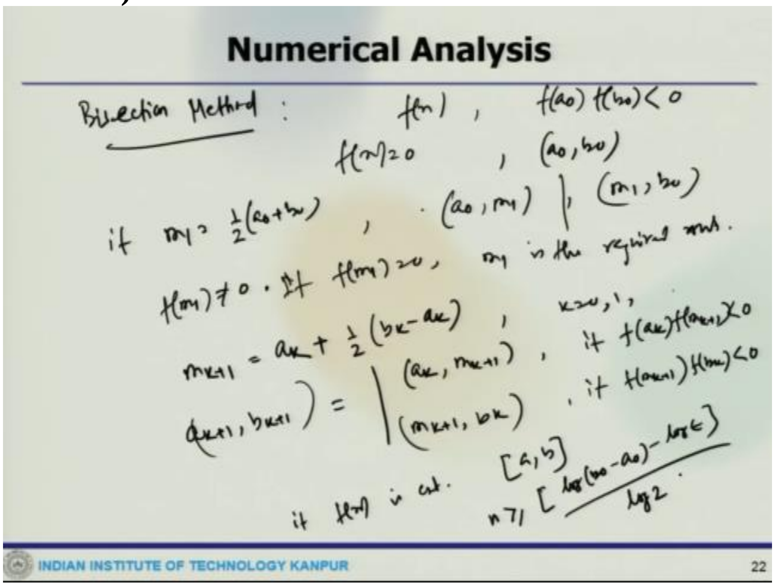

Now, we look at now bisection method so, what we are going to look at here? If the function $f(x)$ which satisfied that

$$f(a_0)f(b_0) < 0$$

then the function $f(x) = 0$ has at least 1 real root and an odd number of real roots in the interval of (a_0, b_0) now, if m_1 is the midpoint of this interval, then the root will lie either in the interval a_0, m_1 or in the interval m_1, b_0 so, either of this interval the root will lie provided that

$$f(m_1) \neq 0$$

if let us say, $f(m_1) = 0$.

Then m_1 is the required root repeating this procedure the number of times we obtained the bisection method, so, like

$$m_{K+1} = a_K + \frac{1}{2}(b_K - a_K)$$

where K goes to 0, 1, 2 and such that were $(a_{K+1}, b_{K+1}) = (a_K, m_{K+1})$ if $f(a_K)f(m_{K+1}) < 0$ and (m_{K+1}, b_K) if $f(m_{K+1})f(b_K) < 0$. we take the midpoint of the last interval as an approximation to the root.

So, this method always converges if $f(x)$ is continuous in the interval a and b which contains the root if an error tolerance in epsilon is prescribed in the approximate number of iteration required maybe also found out like n which would be greater than like

$$n \geq \frac{[\log(b_0 - a_0) - \log \epsilon]}{\log 2}$$

so, this is what one get.

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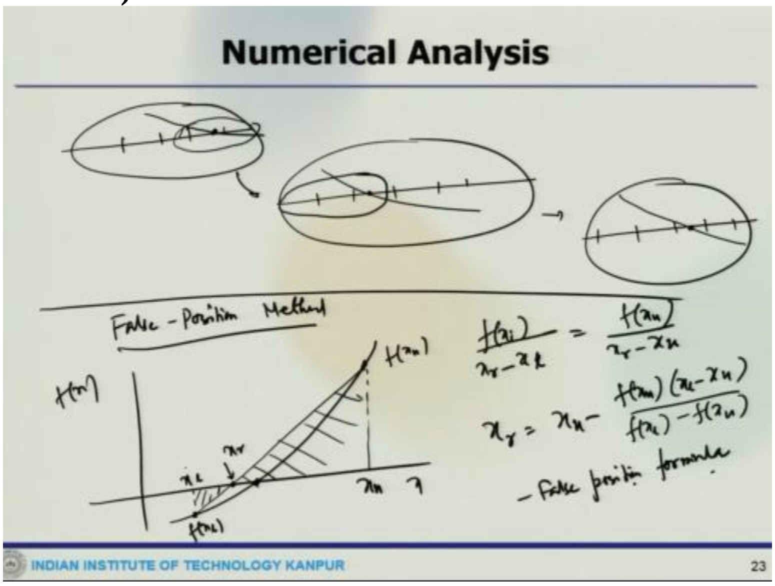

So, it is just like and if you see graphically what happens you have a like this and you have intersection like that and the function process like that. So, this becomes then again you can see that so, that is how the function goes like that. So, this is what it is and then finally, we can approximate the root. So, this process like that, so, that is a number of times it goes and you can find out.

Now so, obviously the termination criteria error one can estimate and estimate the number of iterations which is required. Now, this is quite simple to implement in like now, another thing which could be there is called the false position method, which is called the bisection is perfectly valid for determining roots, it’s a brute force approach is relatively inefficient. So, false position is an alternative based on graphical insight.

But obviously, there are some shortcomings on bisection method, which is the dividing the interval between that lower bound to upper bound into an equal half. Now, the intersection of the line with x axis represent some input. So, we are trying to find out some false position method and like if you say, this is the graphical representation of that and this is how the function goes. So, this here is a one point this comes there this goes there.

So, this is $f(x)$ upper bound this x_u this is x_r this is x lower bound $f(x_1)$. So, we can see this now, so, we can use these similar triangles, the intersection of the straight line with the x axis can be estimated at

$$\frac{f(x_i)}{x_r - x_l} = \frac{f(x_u)}{x_r - x_u}$$

now, which we can now can be solved and after solving what will get

$$x_r = x_u - \frac{f(x_u)(x_l - x_u)}{f(x_i) - f(x_u)}$$

So, this is called false position formula and the value of x_r which is computed here replaces the whichever of the 2 initial cases $x_l \; or \; x_u$ is a functional value with the same sign.

So, this way the values of x_l and x_l the lower bound here and the x_u always bracket the true root the process is repeated until the true root is estimated adequately. So, this is called the false position method. Now, there are some pitfalls this would seem to always be bracketing method for preference, but there are cases where it performs well. In fact, if the function is a particular series function, sometimes it may now there are also modified false method or which can be used. Now, we can go to some fixed point iteration methods and then find out the things where this kind of or there is another method which one can talk about is that.

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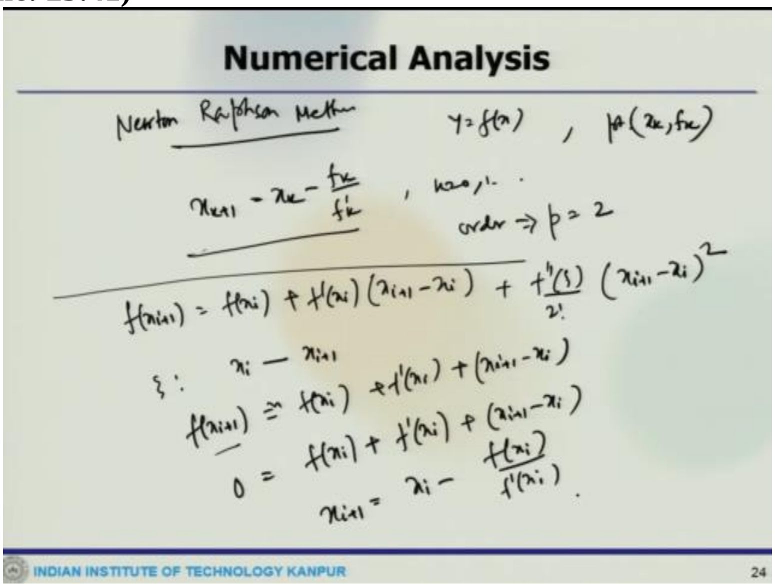

So, there are so, this is like secant method or Newton Raphson method. So, these are fixed point iteration methods which one can find out the let us first talk about the Newton Raphson method. So, what happens in this method, we approximate the graph of function $y = f(x)$ in the neighbourhood of the root by tangent to the curve at the point which is (x_k, f_k) and take this point intersection with the next x axis at the next intersection.

So, the method this is again as a fixed point method so one can write

$$x_{k+1} = x_k - \frac{f_k}{f'_k}$$

K goes from 0, 1, 2 and the order here is that order of this method is p = 2. So, this method requires one function evaluation and one first derivative part iteration. So, this is what so, Newton Raphson method it does. Now, here I mean like there could be all so, some sort of a now, one can do the kind of an either analysis of this Newton Raphson method.

So, we can, let us say, we write the formula like

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \cdots$$

So, ξ lies between the interval between $x_i \; to \; x_{i+1}$. So, this is where ξ lie now, the first derivative we can approximate that if

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

now, at the intersection of the x axis if x i plus would be equal to 0, so, this would be 0. So, what we write that

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

So, this is what we know which is identical to the equation that we have written for the x_i now, this is what do we have derived for Newton Raphson. Now, the Taylor series can be used to estimate the error of this particular formula and this can be done by employing that exact Taylor series can be employed and an exact result would be of obtained.

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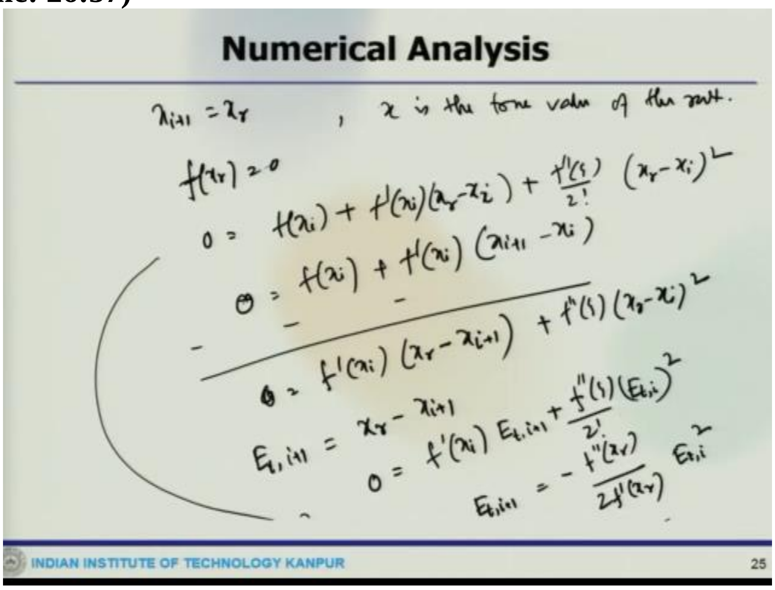

Let us say for that we say x_{i+1} is x_r, where x is the true value of the root. So, substituting this what do we have $f(x_r)$ is 0, so, then what we can write that

$$0 = f(x_i) + f'(x_i)(x_r - x_i) + \frac{f''(\xi)}{2!}(x_r - x_i)^2$$

Now, here we can subtract this expression like this is what we have got in the previous phase let

$$0 = f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

So, if we subtract this what we get is that the E total error.

So, rather we can let us say we will write one more step and then

$$0 = f'(x_i)(x_r - x_{i+1}) + \frac{f''(\xi)}{2!}(x_r - x_i)^2$$

So, what the error would be that

$$E_{t,i+1} = x_r - x_{i+1}$$

if that is the case, then this equation we can rewrite is that

$$0 = f'(x_i)E_{t,i+1} + \frac{f''(\xi)}{2!}\left(E_{t,i}\right)^2$$

Then this guy can be rearranged that this is

$$E_{t,i+1} = -\frac{f''(x_r)}{2f'(x_r)}\left(E_{t,i}\right)^2$$

So, error is roughly proportional to the square of the previous error so, this means that the number of correct decimal places approximately doubles with the iteration. So, this is referred to as a quadratic convergence. And this is one of the important things that one has to, now the other pitfall would be that though this Newton Raphson is quite efficient, there are situation where it performs poorly.

So, the special case like when you have multiple roots, which we will talk about slightly later, that time, the Newton Raphson actually does not do well or cannot perform properly. Now with and so, this is what would happen when you look at the Newton Raphson in that kind of situation where it closes.

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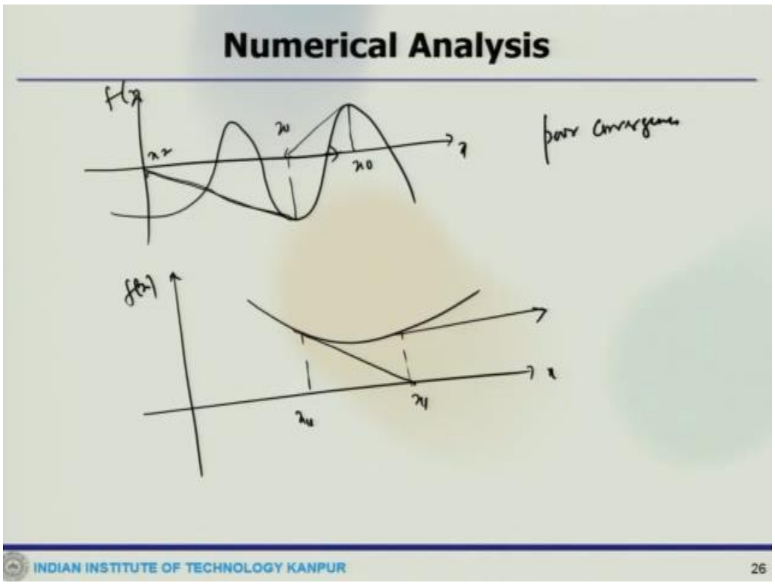

So, I mean, some of this poor convergence situation is that you can see like for sorry, the function could be like this x, if x is there, if you have a function like this. So, this is one of the approximate which is x_1, this is x_0, then it could go to second approximates, which is x_2. So, this is a poor convergence of Newton Raphson or the function could be looking like this. So, these are some of the example when Newton Raphson could be showing poor convergence.

So, the first tangent come here, which is x_1, this is our initial value, then you can see this can go like this. So, these are the situation where Newton Raphson cannot be very handy. So, that is what 1 point iteration of Newton Raphson does so, I will kind of stop here and continue the other methods in the next session.