Computational Science in Engineering

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Lecture – 29
Numerical Analysis

So let us continue the discussion on root finding so we have looked at how to find roots through direct method and the iterative method.

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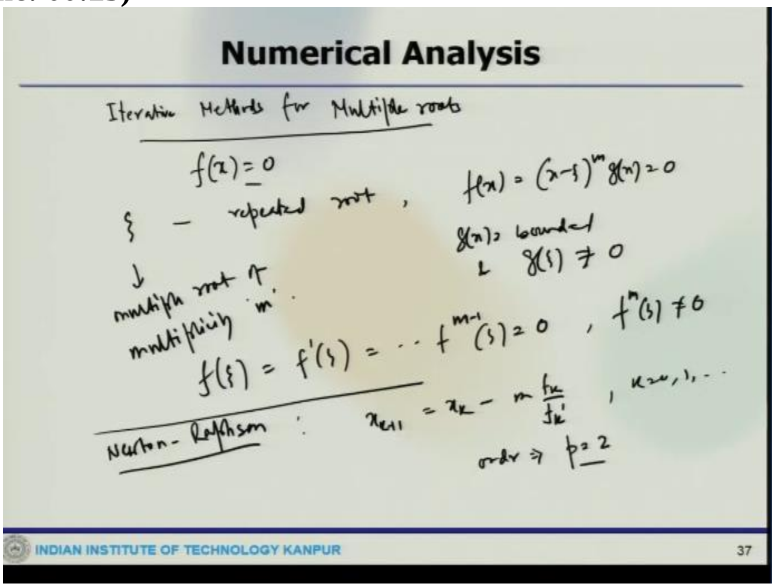

Now today we are going to discuss about something else which is on multiple roots so we will look at the iterative method for multiple roots. So, let us say you have an equation which is like an equation is $f(x) = 0$ and if ξ the root ξ is in a repeated root. So, what we can write

$$f(x) = (x - \xi)^m g(x) = 0$$

Now, g x would be obviously bounded and on top of that, the $g(x) \neq 0$. So, the root ξ called a multiple root of multiplicity m.

Now we obtain the equations, which is like if

$$f(\xi) = f'(\xi) = \cdots = f^{m-1}(\xi) = 0$$

And

$$f^m(\xi) \neq 0$$

So now so far whatever we have discussed there while determining the multiple roots, so they do not retain their order while determining a multiple root and the order is reduced at least by one. So, if the multiplicity of m of a root is known in advance, then we use some different methods like let us say we can do some Newton Raphson.

Similarly, what we have done like they are done in this, when you have multiple roots or rather the multiplicity of a particular root, then the Newton-Raphson becomes like

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

where k is 0 1 2 like that and the order of this particular method would be second order. So, it does not hurt too much, because you still achieve the second order accurate things.

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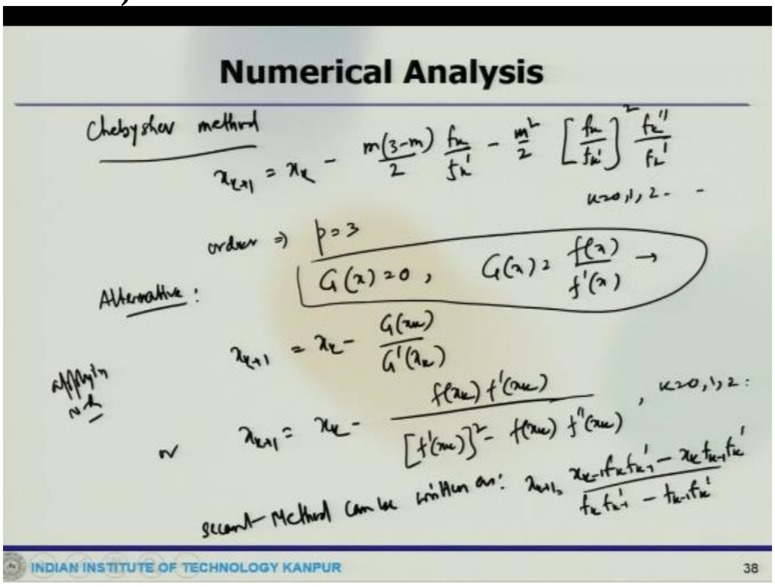

Similarly, one can write the Chebyshev method so, in that case the function which is evaluated will be

$$x_{k+1} = x_k - \frac{m(3-m)}{2}\frac{f_k}{{f_k}'} - \frac{m^2}{2}\left[\frac{f_k}{{f_k}'}\right]^2\frac{{f_k}''}{{f_k}'}$$

for k goes from 0 1 2 so on and the order of this particular method is p = 3 or an alternative way one can write like we applied the previously that we have discussed let us say we define a equation

$$G(x) = 0$$

where

$$G(x) = \frac{f(x)}{f'(x)}$$

So now it has a $G(x)$ has some simple root design regardless of the multiplicity of the root $f(x) = 0$. So, the Newton-Raphson when we apply Newton-Raphson it becomes so applying Newton-Raphson we get

$$x_{k+1} = x_k - \frac{G(x_k)}{G'(x_k)}$$

or one can rewrite this

$$x_{k+1} = x_k - \frac{f(x_k)f'(x_k)}{[f'(x_k)]^2 - f(x_k)f''(x_k)}$$

so, where k is 0 1 like that 2. So, now, similarly, for this particular equation, what we have here like this the secant method can be written as like

$$x_{k+1} = \frac{x_{k-1}f(x_k)f'(x_k) - x_k f(x_{k-1})f'(x_k)}{f(x_k)f'(x_{k-1}) - f(x_{k-1})f'(x_k)}$$

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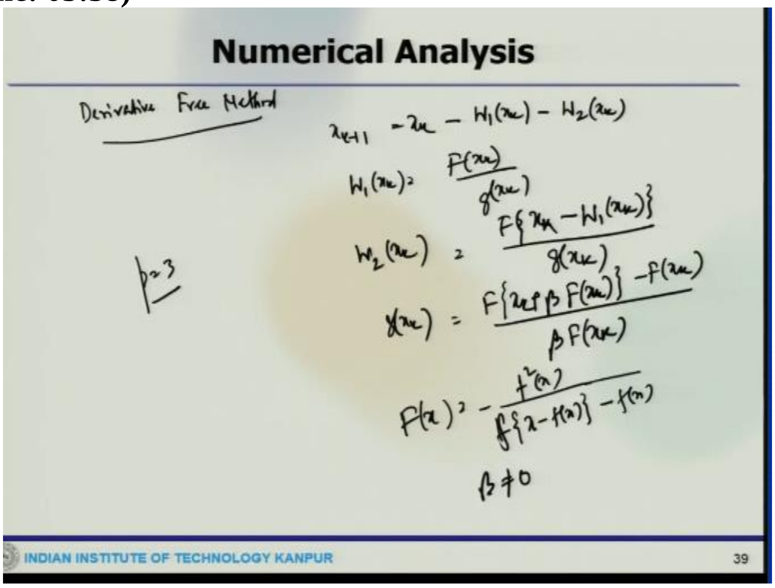

So, this is how you can write and similarly, you can write the like derivative free method so, where you write

$$x_{k+1} = x_k - W_1(x_k) - W_2(x_k)$$

And

$$W_1(x_k) = \frac{F(x_k)}{g(x_k)}$$

and

$$W_2(x_k) = \frac{F\big(x_k - W_1(x_k)\big)}{g(x_k)}$$

and

$$g(x_k) = \frac{F\big(x_k + \beta F(x_k)\big) - F(x_k)}{\beta F(x_k)}$$

and

$$F(x) = \frac{f^2(x)}{f\big(x - f(x)\big) - f(x)}$$

So, here beta obviously is not equals to 0, which is an arbitrary constant so, this requires 6 points on evaluation per iteration and the order of this particular method is also part of them. So, if you see when you have multiple roots, these are the things what you can write like for different approaches.

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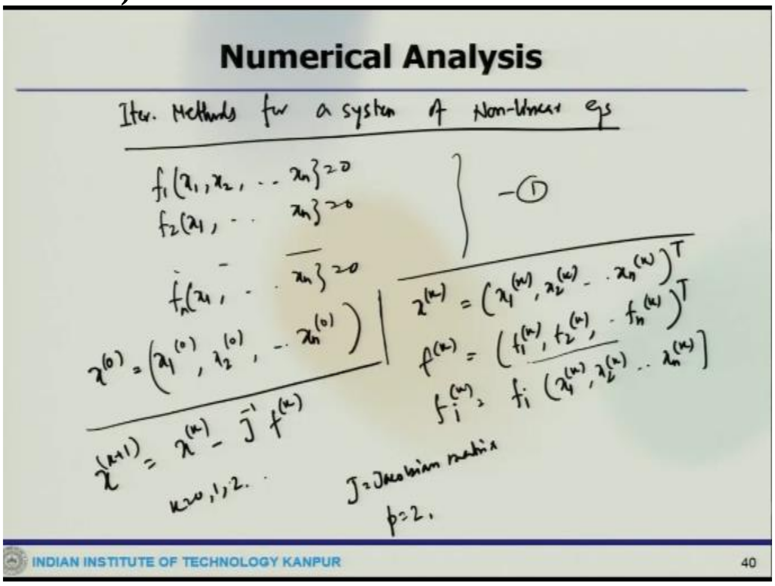

Now, we look at the iterative methods for a system of nonlinear equations so now, as we have done the discussion now, we are going to a system of nonlinear equation let us say given a system of equations, we can write

$$f_1(x_1, x_2, \ldots, x_n) = 0$$
$$f_2(x_1, x_2, \ldots, x_n) = 0$$
$$f_n(x_1, x_2, \ldots, x_n) = 0$$

so, let us say system 1. Now, starting with the initial approximation, which is given at

$$x^{(0)} = \left(x_1{}^{(0)}, x_2{}^{(0)}, \ldots, x_n{}^{(0)}\right)$$

we obtain the sequence of iterations or iterates using the Newton Raphson method.

So, what we can write like if we do the sequence of iteration where we can write

$$x^{(k)} = \left(x_1{}^{(k)}, x_2{}^{(k)}, \ldots, x_n{}^{(k)}\right)^T$$

So, what do we write for Newton-Raphson as:

$$x^{(k+1)} = x^{(k)} - J^{-1} f^{(k)}$$

where k is 0 1 2 so on and $x^{(k)}$ given like that,

$$f^{(k)} = \left(f_1{}^{(k)}, f_2{}^{(k)}, \ldots, f_n{}^{(k)}\right)^T$$

And

$$f_i^{(k)} = f_i\left(x_1^{(k)}, x_2^{(k)}, \dots, x_n^{(k)}\right)$$

where J is the Jacobean matrix and the functions f_1, f_2, f_n these are evaluated.

So, these are the function which are actually evaluated at point $x_1, x_2, \dots, x_n$ like that. So, the convergence of this method which is also is second order, so now, this is what you get. Now, the other thing which may appear is if you have complex roots then what happens?

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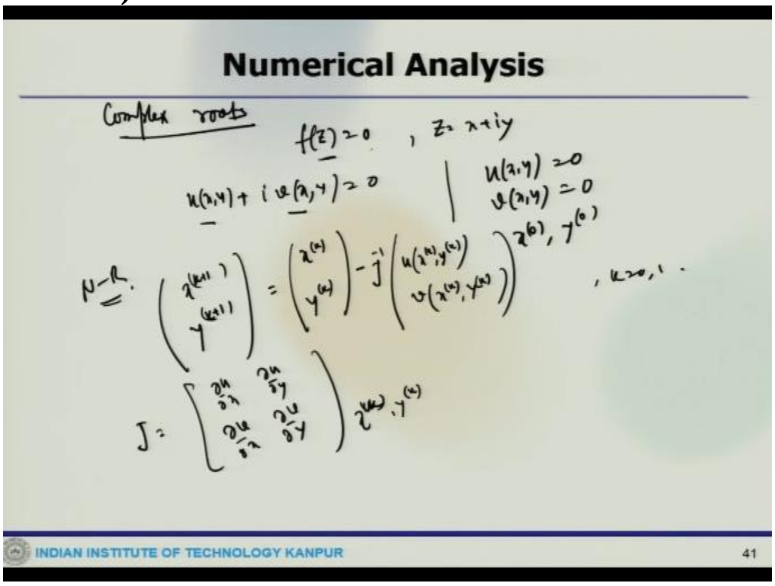

So let us say if you have complex roots, we have been given an equation which is $f(z) = 0$, where $z = x + iy$. So, this equation we can write in the form like

$$u(x, y) + iv(x, y) = 0$$

where $u(x, y)$ and $v(x, y)$ are the real and imaginary part of the $f(z)$ itself. So, the problem of finding this complex root $f(z) = 0$ is equivalent to finding the solution x y of system of 2 equations like $u(x, y) = 0$, $v(x, y) = 0$ and the initial condition would be $x^{(0)}, y^{(0)}$.

So, we can find the series of sequence of iterates like we can write by using Newton-Raphson what we can write is like

$$\begin{pmatrix} x^{(k+1)} \\ y^{(k+1)} \end{pmatrix} = \begin{pmatrix} x^{(k)} \\ y^{(k)} \end{pmatrix} - J^{-1} \begin{pmatrix} u(x^{(k)}, y^{(k)}) \\ v(x^{(k)}, y^{(k)}) \end{pmatrix}$$

where k goes from 0 1 2 like that and the Jacobean is given as

$$J = \begin{bmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial x} \end{bmatrix}_{x^{(k)}, y^{(k)}}$$

So, this is the Jacobian so, the thing which we are written here we can this is one way one can look at it, but alternatively one can directly apply the Newton-Raphson to this particular equation.

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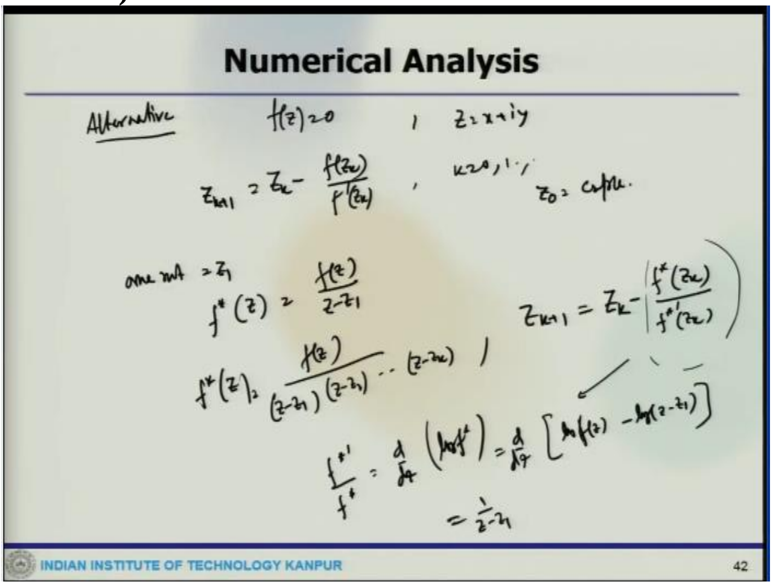

So, if we applied directly to the alternative approach, one can think about that directly applying the Newton-Raphson to these particular equations where $z = x + iy$, so, if we apply directly this that we can write

$$z_{k+1} = z_k - \frac{f(z_k)}{f'(z_k)}$$

Where k= 1 2 like that. Now, this is what uses complex arithmetic now, the initial approximation here is it not is given that is also happens to be complex and then the secant method can also be applied using complex arithmetic.

Now, once finding the one root which is let us say z_1 then we can apply this Newton method for the deflated polynomials like

$$f^*(z) = \frac{f(z)}{z - z_1}$$

So, this can be repeated after finding every root. So, if k roots are already obtained then iteration can be applied on the function like

$$f^*(z) = \frac{f(z)}{(z - z_1)(z - z_2) \dots (z - z_k)}$$

and the new iteration of what we can write

$$z_{k+1} = z_k - \frac{f^*(z_k)}{f^{*\prime}(z_k)}$$

Now, the competition of this particular quantity

$$\frac{f^{*\prime}}{f^{*}} = \frac{d}{dz}(\log f^{*}) = \frac{d}{dz}[f(z) - \log(z - z_1)] = \frac{1}{(z - z_1)}$$

so, that is what you get.

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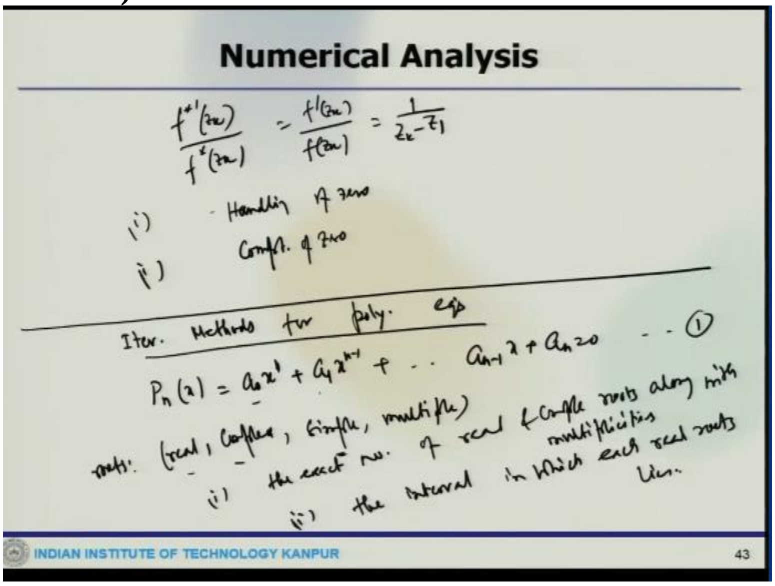

Hence, the computations are carried out like

$$\frac{f^{*\prime}(z_k)}{f^{*}(z_k)} = \frac{f'(z_k)}{f(z_k)} = \frac{1}{(z_k - z_1)}$$

So, there are some precautions one has to take like number 1 any 0 often by using the deflated polynomial should be refined by applying Newton's method. So, to original polynomial with the 0 as the starting approximation that is

i) Handling of zero

ii) Computation of zero

So, the computation of 0 so, the 0 should be so, this is how one can get these things when you have some complex roots. Now, we will talk about none slightly more about like similarly iterative methods for polynomial equation. Now, we are slowly increasing the order of complexity and polynomial equation. So, what it says that whatever we have so, far discussed can be directly applied to obtain the roots of a polynomial of degree n like if it is

$$P_n(x) = a_0x^n + a_1x^{n-1} + \cdots + a_{n-1}x + a_n = 0$$

Let us say equation 1 for are all these $a_0, a_1, \ldots, a_n$ these are the real numbers very often we are interested to determine all the roots whether it is with could be real, could be complex, could be simple root or multiple roots. So, we have already seen all the processes or the methods that can find real root, complex root, simple root or multiple roots. So, then what do we need to know

i) the exact number of real and complex roots along with their multiplicities

ii) the interval in which each real roots lies

so, these are the things that one has to take care so, then what we can often using the Sturm sequences that.

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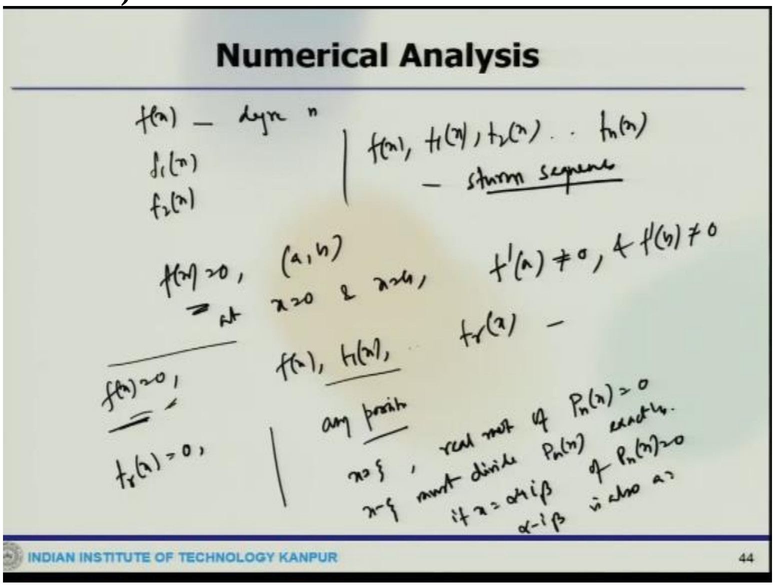

Let us $f(x)$ be the given polynomial of degree n an $f_1(x)$ denotes first order derivative, its first order derivative, then what $f_2(x)$ the remainder of $\frac{f'(x)}{f_1(x)}$ with the reverse sign and $f_3(x)$ is the remainder of $\frac{f_1(x)}{f_3(x)}$ like this. So, until we get the constant number is often the sequence of these functions like

$$f(x), f_1(x), f_2(x), \dots, f_n(x)$$

is called a Sturm sequence.

And the number of real roots for the equation $f(x) = 0$ in a and b equals the difference between the number of sign changes in the Sturm sequence of $f(x) = 0$ sequence at x = a and x = b provided $f'(a) \neq 0$ and $f'(b) \neq 0$. So, one has to note that if any function in the Sturm sequence becomes 0 for some value of x will give it to the sign of the immediately preceding term. So, what if $f(x) = 0$ has multiple roots, we obtain the Sturm sequence like

$$f(x), f_1(x), f_2(x), \dots, f_r(x)$$

And in this case, $f_r(x)$ will be the constant, since $f_r(x)$ gives the greatest common divisor of $f(x) and\ f'(x)$, the multiplicity of root $f(x) = 0$ is one more than the root of a $f_r(x) = 0$. So, we have done a new time sequence by dividing all the function like

$$f(x), f_1(x), f_2(x), \dots, \frac{f_r(x)}{f_r(x)}$$

and using that sequence, you determine the real number of real roots of the equation $f(x) = 0$ and the same way one can take into account the multiplicity of these $f(x) = 0$.

Now, one thing is that while obtaining this Sturm sequence, any positive constant common factor in any Sturm function $f_i(x)$ can be so that has to be neglected. Since the polynomial has degree in so it must have exactly n roots, the number of complex roots equals to the n number of real roots, that the real root of multiplicity M is counted as m times. Let us say, $x = \xi$ is a real root of $P_n(x) = 0$, then $x - \xi$ must divide $P_n(x)$ exactly. So also, if $x = \alpha + i\beta$ is a complex root of $P_n(x) = 0$, then the complex conjugate $\alpha - i\beta$ is also a root.

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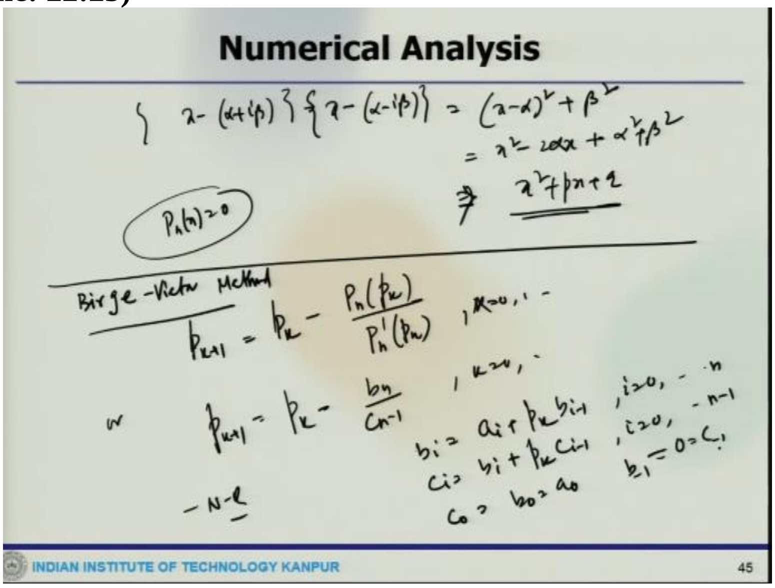

So, what we can write like that,

$$\{x - (\alpha + i\beta)\}\{x - (\alpha - i\beta)\} = (x - \alpha)^2 + \beta^2$$

So, this is going to be

$$x^2 - 2\alpha x + \alpha^2 + \beta^2$$

which is going to be

$$x^2 + px + q$$

something like that where p and q must divide by $P_n(x)$ exactly so, this quadratic factor may have a pair of real roots or pair of complex roots. Hence, the iterative method for finding the real and complex roots of $P_n(x) = 0$ are based on the philosophy of extracting linear and quadratic factor of $P_n(x)$.

Now, we assume that or rather assuming that $P_n(x)$ is complete the polynomial then it has n + 1 terms, if the terms is not present to introduce it today, we can introduce that on with proper replacement with sort of an 0. Now, we will discuss different approaches or methods like first one is that Birge-Vieta method. So, in this case, we seek to determine the real number P such that x - p becomes a factor of $P_n(x)$ starting with P(0).

So, you can find out the sequence of iteration like p_k so, this is let us say

$$p_{k+1} = p_k - \frac{p_n(p_k)}{p_n{}'(p_k)}$$

where k = 0 1 like this or one can write

$$p_{k+1} = p_k - \frac{b_n}{C_{n-1}}$$

so, k = 0 1 2 like that, which is also a sort of an Newton-Raphson method. Now, the values of $b_n \; and \; C_n$ are often from the recurrence relation, like

$$b_i = a_i + p_k b_{i-1}$$

where i = 0 to n,

$$C_i = b_i + p_k C_{i-1}$$

where i = 0 to n - 1 and

$$C_0 = b_0 = a_0$$

and

$$b_{-1} = 0 = C_{-1}$$

So, we can also kind of obtain by using synthetic division method.

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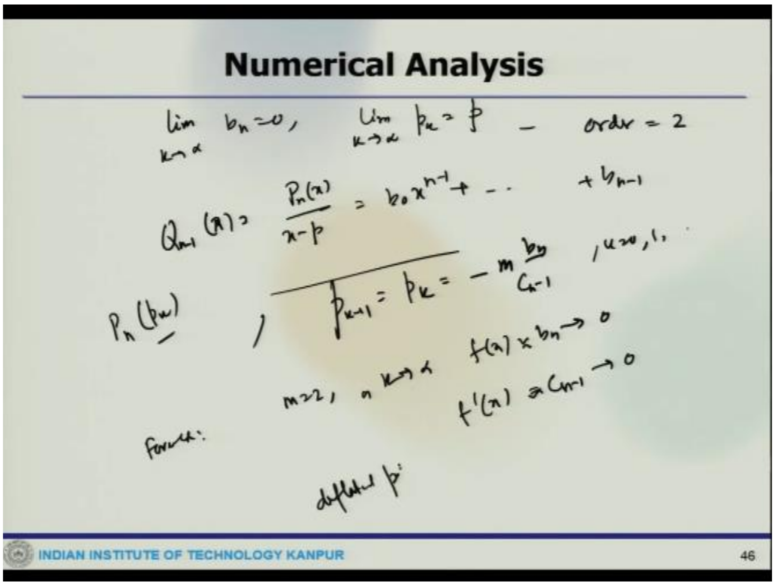

So that is another option that we can have a now when p has been so, what we have that when there is a limit

$$\lim_{k\to\infty} b_n = 0$$

and in the limit,

$$\lim_{k\to\infty} p_k = p$$

so, the order of this method is also the order is second order. So, now, when p has been like in a synthetic now, P has been determined to desired accuracy, we expect the next linear factor for deflated polynomial like

$$Q_{n-1}(x) = \frac{p_n(x)}{x-p} = b_0 x^{n-1} + \cdots + b_{n-1}$$

so this can also be obtained by first part of the synthetic division.

Now, synthetic division procedure for obtaining b_n is same that honours method for evaluating the polynomial $p_n(p_k)$ which is the most efficient way of evaluating the polynomial. So now, we can exact a multiple root of multiplicity m is in Newton-Raphson where we write

$$p_{k+1} = p_k - m\frac{b_n}{C_{n-1}}$$

for k goes from 0 1 like that. So, in this case also one has to be careful while finding the deflated polynomial for example, m = 2, as k tends to infinity, $f(x)$ becomes b_n which tends to 0 and $f'(x)$ becomes C_{n-1} tends to 0.

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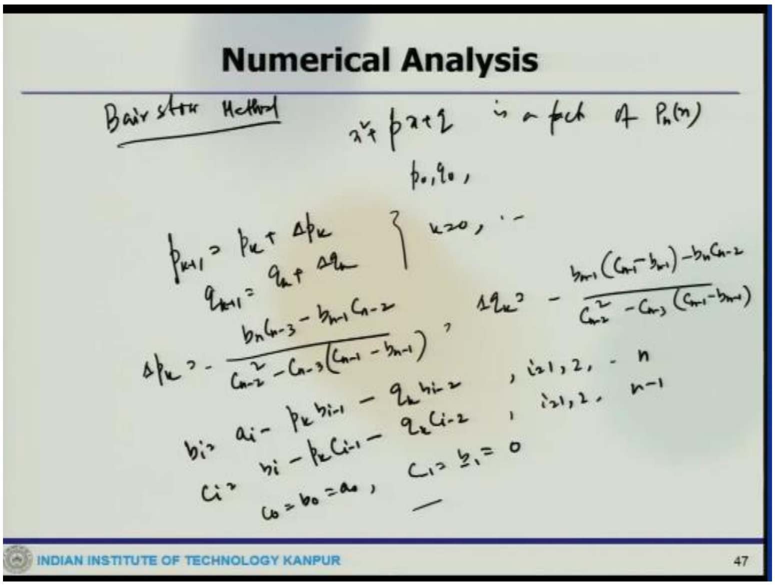

So, now, there are other methods which one can also like use for example, Bairstow method with can also be so, this method is used for find to real numbers p and q such that

$$x^2 + px + q$$

is a factor of $p_n(x)$. Now, we starting with p_0 and q_0 and iterate over p_k and q_k. So, what we can get is that

$$p_{k+1} = p_k + \Delta p_k$$

and

$$q_{k+1} = q_k + \Delta q_k$$

where k goes from 0 1 like that and Δp_k is given as

$$\Delta p_k = -\frac{b_n C_{n-3} - b_{n-1} C_{n-2}}{{C_{n-2}}^2 - C_{n-3}(C_{n-1} - b_{n-1})}$$

And

$$\Delta q_k = -\frac{b_n (C_{n-1} - b_{n-1}) - b_n C_{n-2}}{{C_{n-2}}^2 - C_{n-3}(C_{n-1} - b_{n-1})}$$

So, the values of b_i and C_i which are obtain 2 recurrence relation like

$$b_i = a_i - p_k b_{i-1} - q_k b_{i-2}$$

where i goes from 1 to n.

$$C_i = b_i - p_k C_{i-1} - q_k C_{i-2}$$

where i goes 1 to n-1,

$$C_0 = b_0 = a_0$$

and

$$b_{-1} = 0 = C_{-1}$$

So, I mean one can also kind of get these coefficients using the synthetic division.

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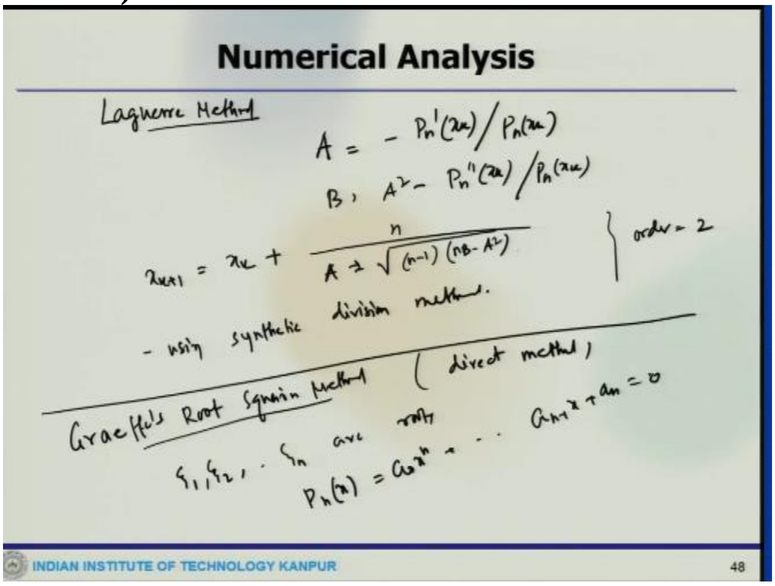

But this is how one can use this method to find the there are other methods like one can use like Laguerre method. So, here we define the parameter like A, which is

$$A = -\frac{p_n{}'(x_k)}{p_n(x_k)}$$

And

$$B = A^2 - \frac{p_n{}''(x_k)}{p_n(x_k)}$$

So, this method which leads to the getting the iteration like

$$x_{k+1} = x_k + \frac{n}{A \pm \sqrt{(n-1)(nB - A^2)}}$$

these parameters are obtained using synthetic division method.

So, the sign in the denominator of the of this particular equation is taken as the sign of A to make the denominator here largest in magnitude and order of this method for convergence is also second order. Now, what we can now look at is that another method which is called Graeffe's root squaring method. So, this is a direct method and it is used to find out all the roots of a polynomial. So, this is a direct method of with real coefficients, the roots could be real and distinct, real and equal or complex we can separate the roots.

And then, so let us say $\xi_1, \xi_2, \xi_3, \ldots, \xi_n$ our roots of equation of this polynomial equation these are roots of this

$$P_n(x) = a_0x^n + \cdots + a_{n-1}x + a_n = 0$$

so, these are the roots of this equation.

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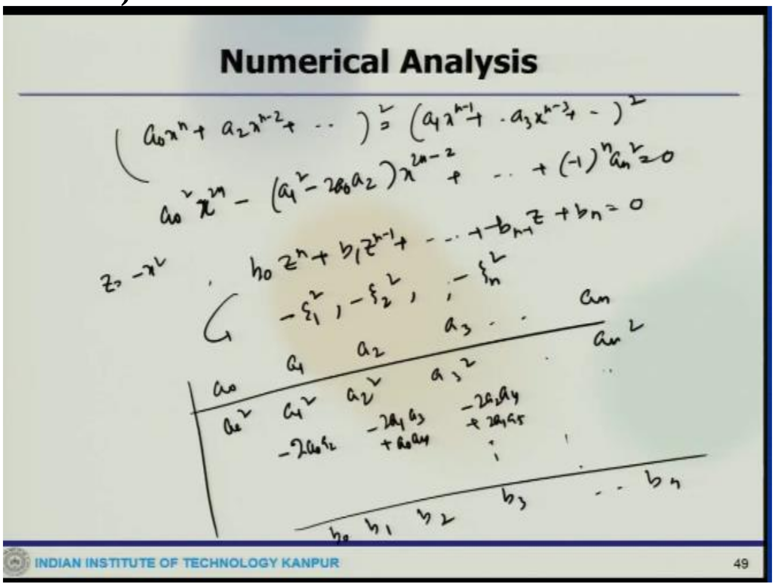

Now, we are separating the even power of x_n squaring, we get

$$(a_0 x^n + a_2 x^{n-2} + \cdots)^2 = (a_1 x^{n-1} + a_3 x^{n-3} + \cdots)^2$$

Now, once we simplify what we get in

$${a_0}^2 x^{2n} - ({a_1}^2 - 2a_0 a_2) x^{2n-2} + \cdots + (-1)^n {a_n}^2 = 0$$

Here we substitute

$$z = -x^2$$

what do we get

$$b_0 z^n + b_1 z^{n-1} + \cdots + b_{n-1} z + b_n = 0$$

So, which has a root this guy has root of $-{\xi_1}^2, -{\xi_2}^2, -{\xi_3}^2, \ldots, -{\xi_n}^2$.

And the coefficients which can be obtained like can one can see like $a_0, a_1, a_2, a_3, \ldots, a_n$ like this is ${a_0}^2, {a_1}^2, {a_2}^2, \ldots, {a_n}^2$. So, how do we find the k + 1 column in this particular table which is a tricky term so you can see the each terms in each column alternated signs starting with the positive sign. So, the first term in the square of the k + 1 coefficient is a k, the second term would be twice of that.

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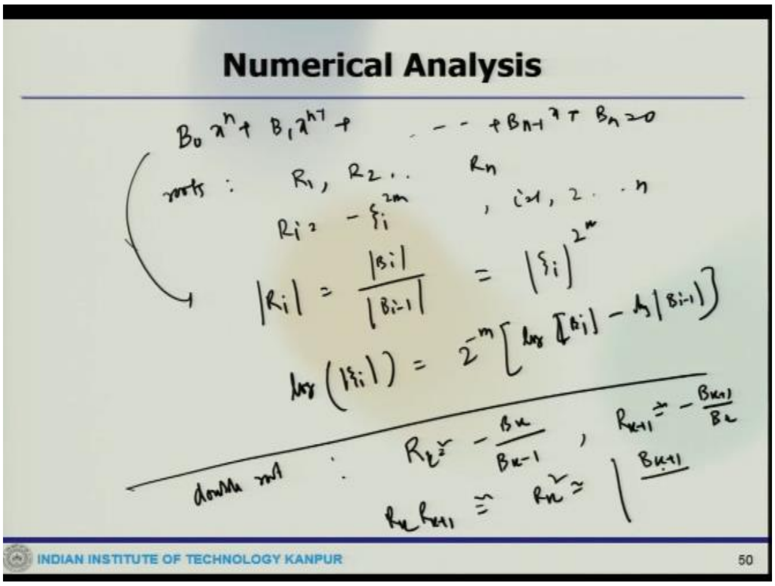

And so, once we repeat that procedure for m times, we can obtain an equation like

$$B_0x^n + B_1x^{n-1} + \cdots + B_{n-1}x + B_n = 0$$

So, what do we get, so the roots are $R_1, R_2, R_3, \ldots R_n$ where $R_i = -\xi_i^{2m}$, i = 1, 2, … n. So, we can obtain from this particular equation that

$$|R_i| = \frac{|B_i|}{|B_{i-1}|} = |\xi_i|^{2m}$$

So,

$$\log|\xi_i| = 2^{-m}[\log|B_i| - \log|B_{i-1}|]$$

So, this determines the magnitude of the roots and substitution this in the original equation with the sign of the root. Now, we can stop squaring process when another starting process produces new coefficients. And after a few squaring actually, the magnitude of the coefficient B_K is half the square of the magnitude of the corresponding coefficient the previous equation, so, which indicates that B_K is a double root we can find the double root by like

$$R_K = -\frac{B_K}{B_{K-1}}$$

and

$$R_{K+1} = -\frac{B_{K+1}}{B_K}$$

where

$$R_K R_{K+1} = R_K^2 = \frac{B_{K+1}}{B_{K-1}}$$

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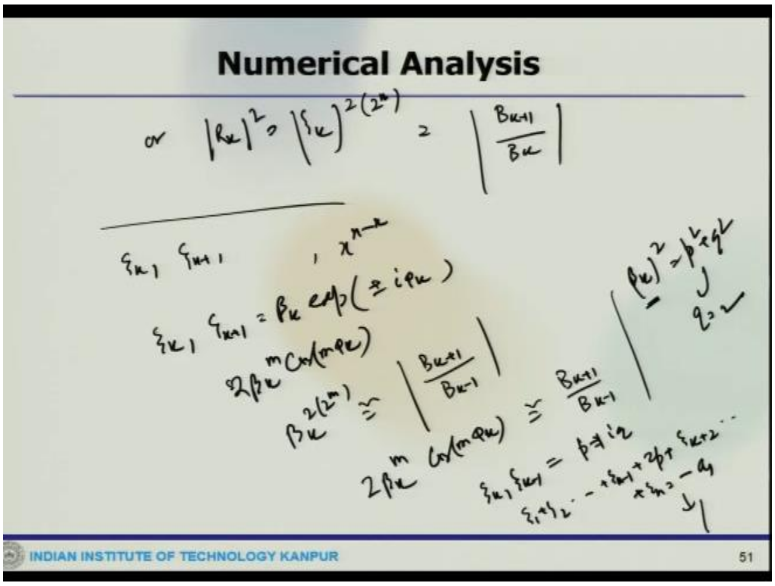

Or one can write

$$|R_K|^2 = |\xi_K|^{2(2^n)} = \left|\frac{B_{K+1}}{B_K}\right|$$

like this so, this gives the magnitude of the double root substitution this in the given equation you can find it sign. So, double root can also be found directly since R_K and R_{K+1} converge to the same root after sufficient squaring. Now, if ξ_K and ξ_{K+1} form a complex pair then this would also cause the coefficient of x^{n-k} in the successive squaring to fluctuate both in magnitude and sign.

So, if $\xi_K, \xi_{K+1} = \beta_K \exp(\pm i\phi_k)$ is a complex pair we are in the coefficient would fluctuate in magnitude and sign by amount like $2{\beta_K}^m \cos(m\phi_k)$. So, a complex pair can be spotted by such oscillation like for m sufficiently large is the

$${\beta_K}^{2(2^m)} \cong \frac{B_{K+1}}{B_{K-1}}$$

and which will be determined like

$$2{\beta_K}^m \cos(m\phi_k) \cong \frac{B_{K+1}}{B_{K-1}}$$

so, if the equation has only one complex pair.

Then we can first determine all the real roots and the complex pair can be written like

$$\xi_K, \xi_{K+1} = p \pm iq$$

and the sum of the roots would lead to like $\xi_1 + \xi_2 + \cdots$ and so on $\xi_n = -a_1$. So, this will determine P and we also have like ${\beta_K}^2 = p^2 + q^2$. Since magnitude of β_K is already determine these equations provides q.

So, this provides q this provides p so that is how you can find out so, that is pretty much actually gives you an idea of how you can find out roots for I mean when you have real root for a polynomial and the functions are distinct root or complex. So, we will stop here and continue the discussion in the next session.