Computational Science in Engineering

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Lecture - 28
Numerical Analysis

Let us continue the discussion on root finding. So, we have looked at this first simply one is the Newton Raphson, which is a point iterative method. Now, we are going to look at the other one, which is called the Secant Method.

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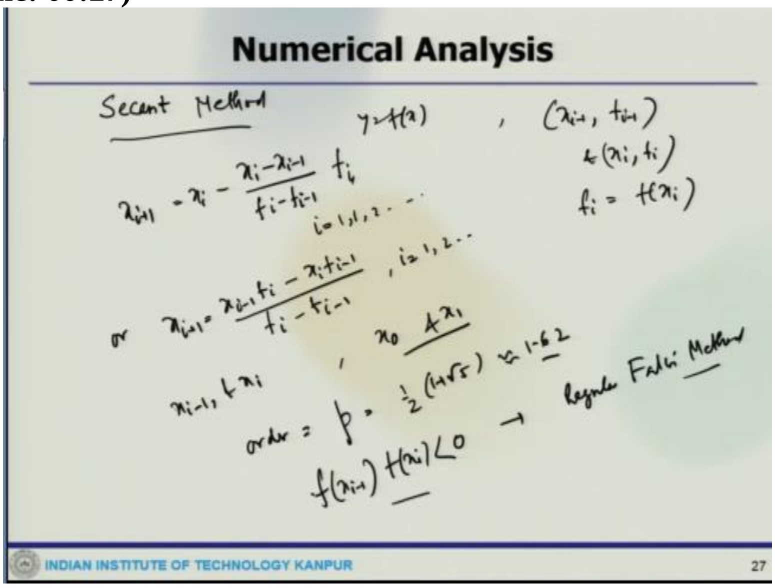

So, in the Secant Method, what it does is that so, basically the some of the potential problem which you see in the Newton Raphson method in the evolution of the derivative, so, although that is not inconvenient for polynomial and many other functions, but there is certain function whose derivative is maybe extremely difficult and inconvenience to evaluate. So, for these cases the derived can be accepted by the backward method.

And so, this is where like we approximate the graph of the function $y = f(x)$ in the neighbourhood of the root by straight line on the secant passing through the points which would be (x_{i-1}, f_{i-1}) and (x_i, f_i). So, here $f_i = f(x_i)$ and take the point of intersection of this line to go for iteration. So, like we can see

$$x_{i+1} = x_i - \frac{x_i - x_{i-1}}{f_i - f_{i-1}} f_i$$

so, here i goes from 1, 2, 3 like that or one can write

$$x_{i+1} = \frac{x_{i-1} f_i - x_i f_{i-1}}{f_i - f_{i-1}}$$

so, that is what one can write.

So, i equals to 1, 2, 3 and where x_{i-1} *and* x_i are two consecutive iterates So, in this particular method we need two initial approximations like x_0 and x_1. So, also this method is called the Chord method and the order of the method is obtained like the order of the method would be

$$p = \frac{1}{2}(1 + \sqrt{5}) \approx 1.62$$

So, this is less than second order and so, this is what one can say and if the approximations are chosen such that

$$f(x_{i-1})f(x_i) < 0$$

for each i, then the method is known that the Regula Falsi Method.

So, that the linear or first order of convergence both these methods require one function evolution per iteration. So, now, one can see this is where the; it can differ and the Secant method could be different from these things.

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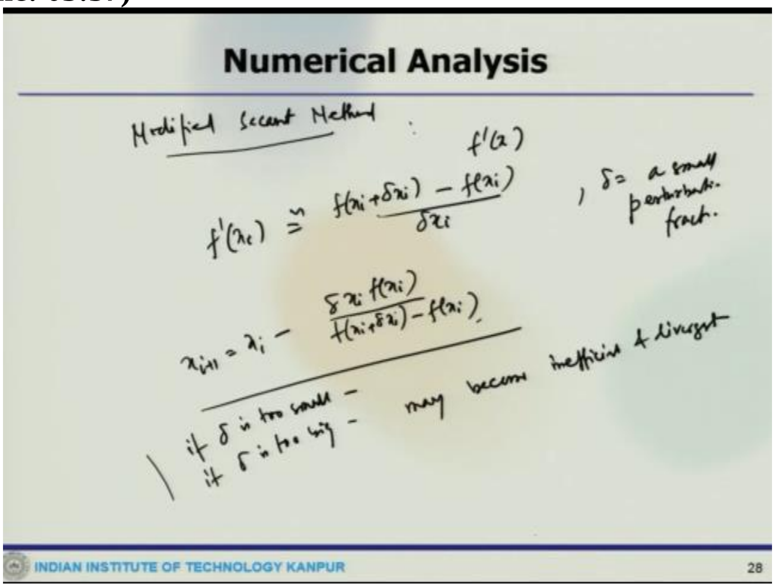

Now, that are like modified Secant method which one can say like sure, I mean this is rather using two arbitrary values to estimate the derivative and alternative approach involves a functional perturbation of the independent variable to find out $f'(x)$. So, one can write which is like

$$f'(x_i) \cong \frac{f(x_i + \delta x_i) - f(x_i)}{\delta x_i}$$

so, where δ is a small perturbation fraction. So, the approximation can be substituted in original formula of the Secant method like one can put it in this.

So, if you substitute in this original formula like f prime derivative then which, what we can get

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

so, this is what you get. So, the choice of delta is not automatic. So, if delta is too small, then the method can be slammed by round off error caused by subtractive cancellation in the denominator of this particular equation or if delta is too big, then the technique can become inefficient and even divergent, so, that is also possible.

However, if the delta is chosen properly or correctly, it provides a nice alternative for cases where evaluating the derivative is difficult and rather developing two initial guesses are inconvenient, like in the original secant method, so, this gives them some sort of an alternatives.

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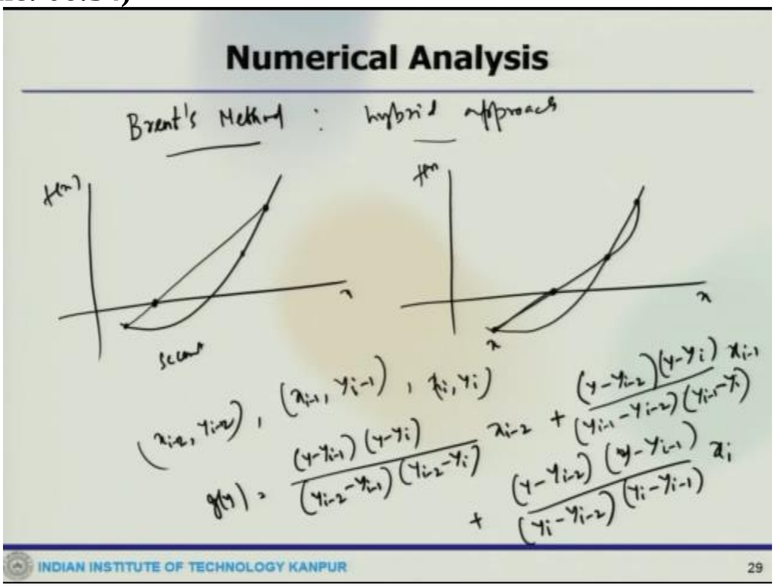

Now, then there is another method which is called the Brent's method. So, this would be kind of a hybrid approach, like it is a I mean, apply the some of this graphical or bracketing approach and then the, probably the one point iteration, so, bracketing technique is just the trusty bisection method whereas two different and one point iteration like secant method or Newton Raphson can be merged. So, here inverse quadratic interpolation is similar in spite of the secant method so, we use that.

So, let us say we have a function like these effects where goes like this and the function goes like this and this is how we go and this is what how you obtain in the secant method, so, this is Secant method approximation, and if you do inverse quadratic interpolation, so, this function will go like this, but what you do? You go like this and you go like that. So, that is called inverse quadratic interpolation.

Now, suppose we have three points in this case, we could determine the quadratic functions like these how it is defined. Now, although this would seem to represent a great improvement, the approach has a fundamental law, it is possible that the parabola might not intersect with the x axis such would be the case when the resulting parabola has complex roots and that could be a problem.

And then the difficulty can be rectified by employing inverse quadratic interpolation. Thus, rather than using a parabola in $f(x)$, so, let us say we have a function like we can, let us say, 3 points are designed as

$$(x_{i-2}, y_{i-2}), (x_{i-1}, y_{i-1}), (x_i, y_i)$$

a quadratic function y that passes through the point can be generated like

$$g(y) = \frac{(y - y_{i-1})(y - y_i)}{(y_{i-2} - y_{i-1})(y_{i-2} - y_i)} x_{i-2} + \frac{(y - y_{i-2})(y - y_i)}{(y_{i-1} - y_{i-2})(y_{i-1} - y_i)} x_{i-1} + \frac{(y - y_{i-2})(y - y_{i-1})}{(y_i - y_{i-2})(y_i - y_{i-1})} x_i$$

So, these forms are called the Lagrange polynomials, the root x_{i+1} corresponds to y_0 which means putting it here.

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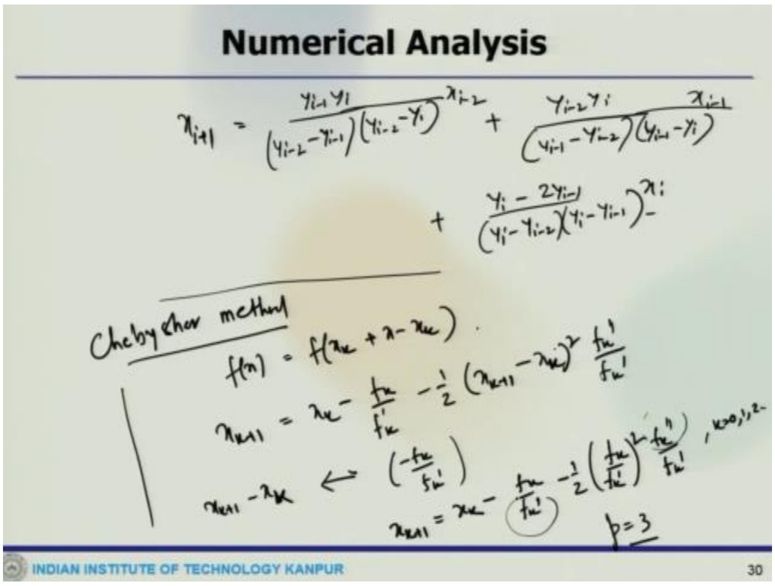

Which gives us that

$$x_{i+1} = \frac{y_{i-1}y_i}{(y_{i-2} - y_{i-1})(y_{i-2} - y_i)}x_{i-2} + \frac{y_{i-2}y_i}{(y_{i-1} - y_{i-2})(y_{i-1} - y_i)}x_{i-1}$$

$$+ \frac{y_i - 2y_{i-1}}{(y_i - y_{i-2})(y_i - y_{i-1})}x_i$$

So, that it can so, now, one can implement this one in any through the programming language, this is just requiring some involvement to find out to the thing. Now, the other thing is that I mean similarly, we can have like this there are some other methods which could be also handy and just to find out for example, we talked about Chebyshev method.

So, here we can write the function

$$f(x) = f(x_k + x - x_k)$$

and approximate effects my second degree Taylor series expansion about x_k where we can get

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

So, you can replace $x_{k+1} - x_k$ on the right hand side here so, this one we can replace by $-\frac{f_k}{f'_k}$ we get that Chebyshev method like

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

where k from 0, 1, 2 something like that the order of this method is 3. So, the method requires 1 function 1 first derivative and 1 second derivative evaluation per iteration.

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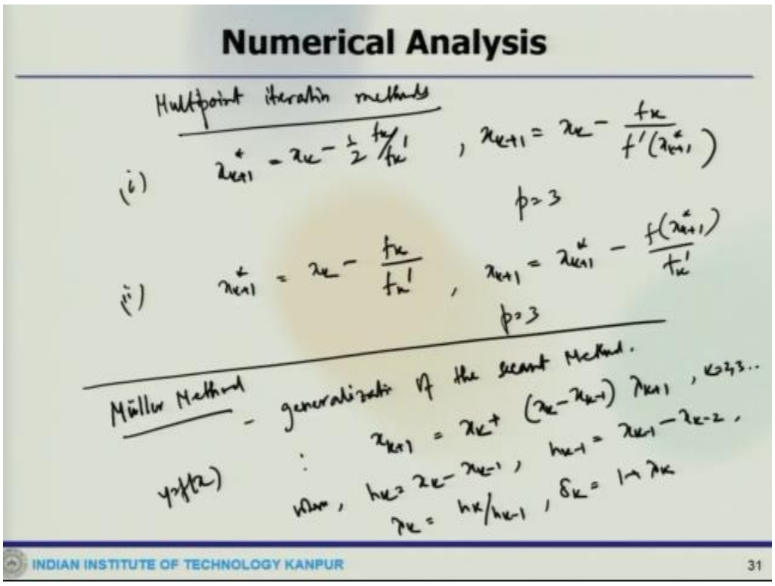

So, here this is the second derivative, this is the first derivative in per iterative and this is now these are single points so, far what we have talked about single point iteration now, there could be multi point iteration methods like so, it is possible to modify like that Chebyshev method and obtain third order iterative methods which do not require the evolution of the second derivative.

So, then we can talk about like we can have 2 different multi point methods like one case it could be

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

which will lead to

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

where the order is third this method requires 1 function it requires 1 function 1 first derivative evaluation at the each time iteration or the second one which could be

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

so that we get

$$ x_{k+1} = {x_{k+1}}^* - \frac{f({x_{k+1}}^*)}{{f'}_k} $$

this also order of third order.

So, this requires 2 function like f_k and $f({x_{k+1}}^*)$ and 1 first derivative evaluation per iteration. So, now we will talk about some other methods like Muller method. So, Muller method one can say that this is a generalization of the secant method here we approximate the graph of the function $y = f(x)$ in the neighbourhood of the root by a second degree curve and take one of its points of intersection with x axis as the next approximation.

So, which means, we can write

$$x_{k+1} = x_k + (x_k - x_{k-1})\lambda_{K+1}$$

where k = 2, 3 and so, on. So, the things which are defined here like

$$h_k = x_k - x_{k-1}$$

$$h_{k-1} = x_{k-1} - x_{k-2}$$

such that

$$\lambda_K = \frac{h_k}{h_{k-1}}$$

And

$$\delta_k = 1 + \lambda_K$$

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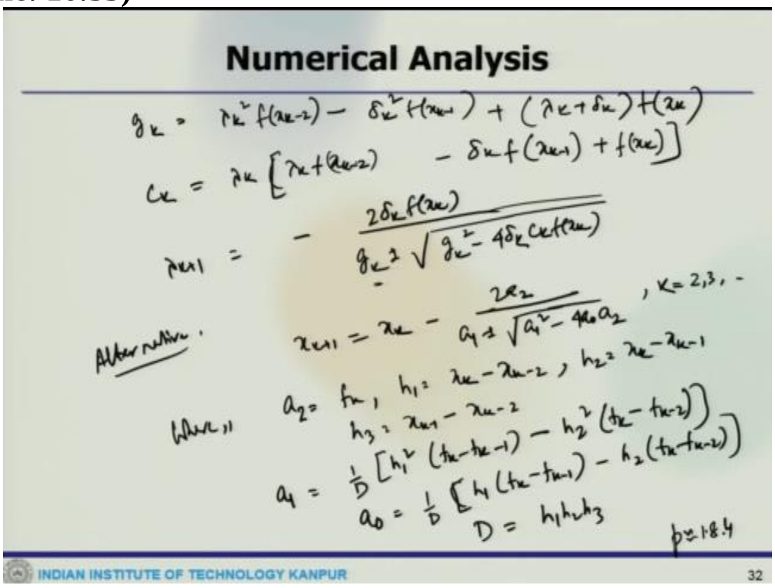

Also, we have

$$g_k = {\lambda_K}^2 f(x_{k-2}) - {\delta_K}^2 f(x_{k-1}) + (\lambda_K + \delta_K) f(x_K)$$

or we get

$$C_k = \lambda_K[\lambda_K f(x_{k-2}) - \delta_K f(x_{k-1}) + f(x_K)]$$

which is like this and

$$\lambda_{K+1} = -\frac{2\delta_K f(x_k)}{g_k \pm \sqrt{{g_K}^2 - 4\delta_K f(x_k)}}$$

so, the sign of the denominator is chosen. So, that λ_{K+1} always has the smallest absolute value that is in the sign of the square root in the denominator is that of g_k.

So, this is one way to write that, or one can write in a alternative way, which is like we can write the method like

$$x_{K+1} = x_K - \frac{2a_2}{a_1 \pm \sqrt{{a_1}^2 - 4a_0a_2}}$$

k = 2, 3 such that where we have like

$$a_2 = f_K$$

$$h_1 = x_k - x_{k-2}$$

$$h_2 = x_k - x_{k-1}$$

$$h_3 = x_{k-1} - x_{k-2}$$

and we get

$$a_1 = \frac{1}{D}\left[{h_1}^2(f_K - f_{K-1}) - {h_2}^2(f_K - f_{K-2})\right]$$

we get

$$a_0 = \frac{1}{D}[h_1(f_K - f_{K-1}) - h_2(f_K - f_{K-2})]$$

and

$$D = h_1h_2h_3$$

So, the sign in that denominator is chosen so that the λ_{K+1} has the smallest absolute value, the sign of the square root is the denominator closes 2 like a_1. So, this method requires 3 initial conditions initial approximation to the root and 1 function evaluation per iteration. And the order of this method is roughly 1.84 or something like that.

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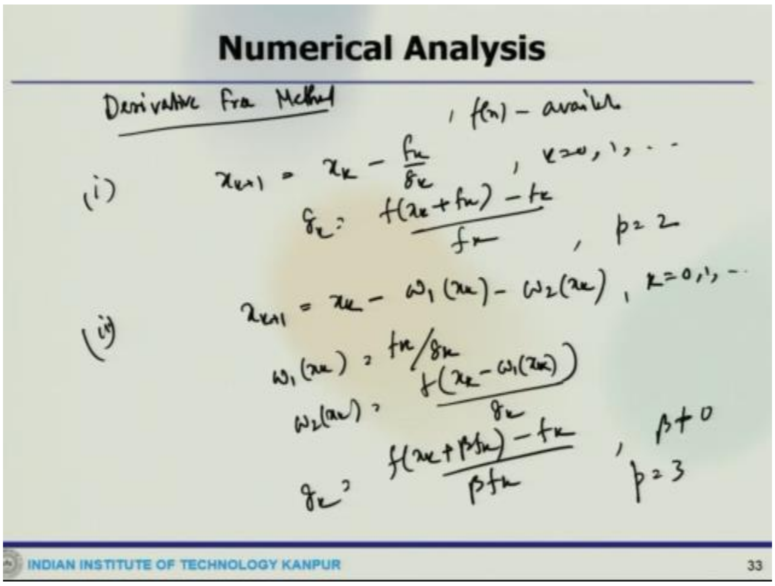

Now, this is what you can see as Muller method. Now, there one can also see some kind of a derivative free method. So, in many practical applications only the data regarding the function $f(x)$ is available. So, in these cases method which do not require the evolution of the derivative which can be very handy. So, there are 2 such kind of methods one way is that one can write

$$x_{K+1} = x_K - \frac{f_K}{g_K}$$

where k goes from 0, 1 so on and g_K is defined as

$$g_K = \frac{f(x_K + f_K) - f_K}{f_K}$$

and the order of this method is 2.

So, this method requires calculation of 2 function at per iteration or the second way one can do that writing

$$x_{K+1} = x_K - \omega_1(x_K) - \omega_2(x_K)$$

where k goes from 0, 1 such that, where you can have

$$\omega_1(x_K) = \frac{f_K}{g_K}$$

and

$$\omega_2(x_K) = \frac{f\left(x_K - \omega_1(x_K)\right)}{g_K}$$

and

$$g_K = \frac{f(x_K + \beta f_K) - f_K}{\beta f_K}$$

So, here beta obviously is not equals to 0, which is arbitrary and the order of method is third order. So, here if you see this requires calculation of 3 functions at 1 iteration.

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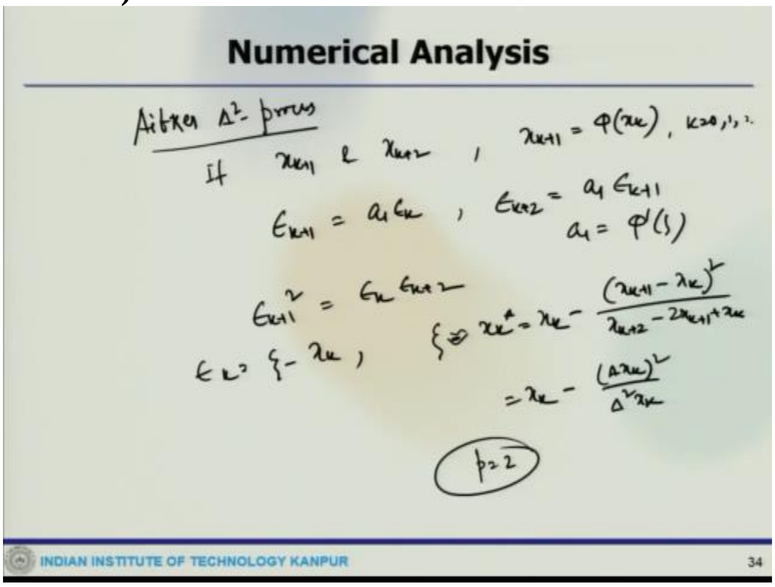

Now, other is that like one can have Aitken delta 2 process. So, if

$$x_{K+1} = x_{K+2}$$

are 2 approximations obtained from general linear iteration method, so, that

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

where k goes from 0, 1, 2 says that, then the error in successive approximation is given by like

$$\epsilon_{k+1} = a_1 \epsilon_k$$

and

$$\epsilon_{k+2} = a_1 \epsilon_{k+1}$$

where

$$a_1 = \phi'(\xi)$$

now, eliminating a one from these 2 equations what we get

$${\epsilon_{k+1}}^2 = \epsilon_k \epsilon_{k+2}$$

Now, we use

$$\epsilon_k = \xi - x_k$$

and what we get ξ is roughly

$$\xi \approx {x_k}^* = x_k - \frac{(x_{k+1} - x_k)^2}{x_{k+2} - 2x_{k+1} + x_k} = x_k - \frac{(\Delta x_k)^2}{\Delta^2 x_k}$$

So, here the order of convergence is 2 or rather second order convergent method.

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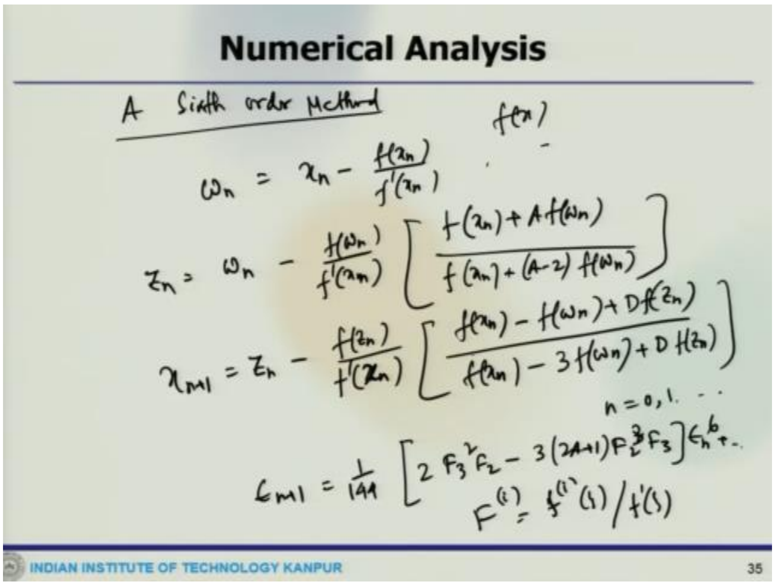

Now, we can look at slightly higher than method like a 6th order method to find out also the root say 1 parameter family of 6th order methods for finding simple zones for effects which required 3 evaluations of $f(x)$ and 1 evaluation of the f prime x which can be given as

$$\omega_n = x_n - \frac{f(x_n)}{f'(x_n)}$$

So, in iteration you get 1 function evolution and then the derivative where one can write

$$z_n = \omega_n - \frac{f(\omega_n)}{f'(\omega_n)}\left[\frac{f(x_n) + Af(\omega_n)}{f(x_n) + (A-2)f(\omega_n)}\right]$$

And

$$x_{n+1} = z_n - \frac{f(z_n)}{f'(x_n)}\left[\frac{f(x_n) - f(\omega_n) + Df(z_n)}{f(x_n) - 3f(\omega_n) + Df(z_n)}\right]$$

which is n = 0, 1 and such that the error term that we can write

$$\epsilon_{n+1} = \frac{1}{144}[2F_3^2F_2 - 3(2A+1)F_2^3F_3]{\epsilon_n}^6 + \cdots$$

the order of the method does not depend on D.

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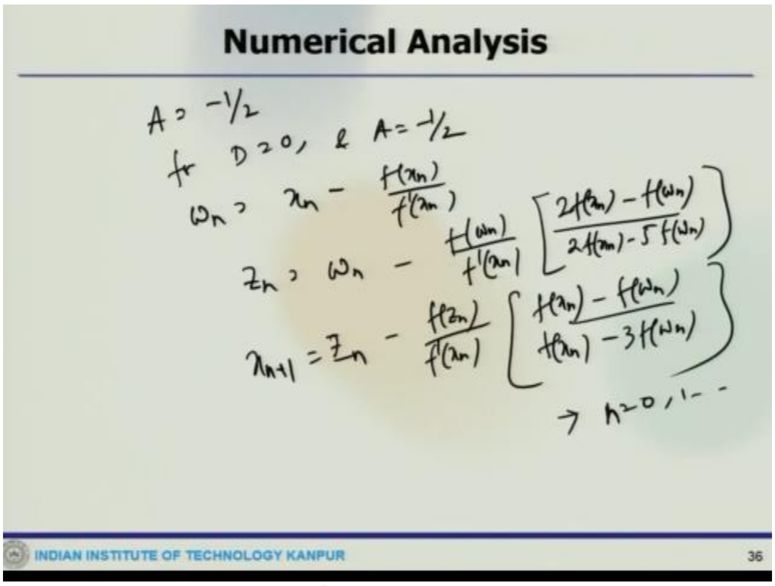

The error term is simplified when $A = -\frac{1}{2}$ the simplified formula for D = 0 and $A = -\frac{1}{2}$ like

$$\omega_n = x_n - \frac{f(x_n)}{f'(x_n)}$$

$$z_n = \omega_n - \frac{f(\omega_n)}{f'(\omega_n)}\left[\frac{2f(x_n) - f(\omega_n)}{2f(x_n) - 5f(\omega_n)}\right]$$

finally,

$$x_{n+1} = z_n - \frac{f(z_n)}{f'(x_n)}\left[\frac{f(x_n) - f(\omega_n)}{f(x_n) - 3f(\omega_n)}\right]$$

where n goes from 0, 1, 2 like that. So, this is the 6th order method which one can have. So, what you can see there are different ways one can find out the roots and there are different, different approaches and every method has its own some of the problems or other advantage and disadvantage.

And now, using the computer and your computational algorithm, these are the mathematical expression one can exactly program that in the computational method or through the computational method or program that in the computational program, which can give you the output. And instead of solving analytically, you can find out through computational approach. So, this is where your mathematical background becomes handy to get a proper numerical method. So, we will stop here and continue the discussion in the next lesson.