Computational Science in Engineering

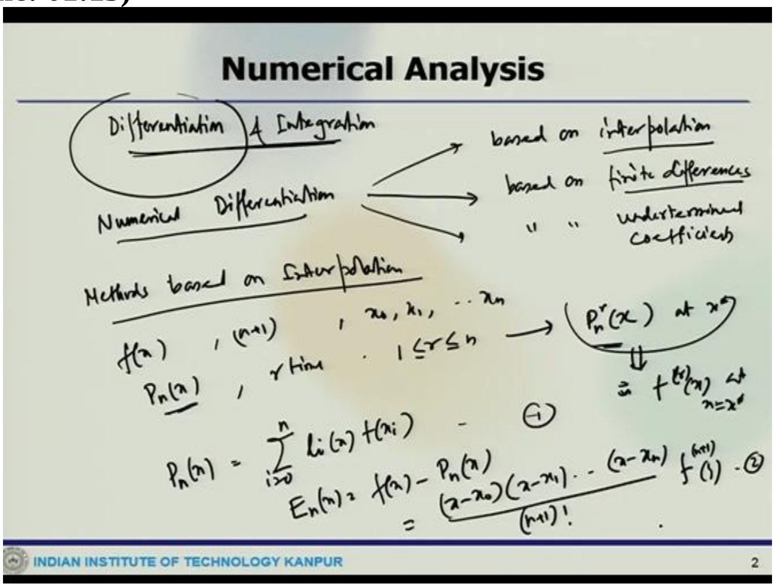
Prof. Ashoke De
Department of Aerospace Engineering
Indian Institute of Technology – Kanpur

Lecture –35
Numerical Analysis

Let us continue the discussion now on the numerical analysis part so far, we have looked at the finding of the roots, whether it is a normal equation and polynomial equation. Then we move to the system of linear equation, which is a kind of connected with the previous discussion when we talked about linear algebra or the matrices and all these things. But this is more like an in point of view of how you implement them as a numerical code where you can solve the linear system like Ax = b.

And then finally, I mean, we have looked at some of the interpolation and approximations which are often used when you actually expand a function are in the polynomial. Now, in this session, actually we are going to talk about a little bit of integration and differentiation, not in very details, but we will touch upon some of the important ways that how one can look at all these and then we move to the solution of the differential equations.

(Refer Slide Time: 01:13)



So, let us start with the differentiation and integration so, the let us say if a function explicitly or defined that set up some points, we can find out all these for differentiation and integration. Now, first, we will start with the numerical differentiation, so when we talk about numerical differentiation, actually there are methods which can be applied, there are 3 ways one can do that, one is the which are the methods which are based on interpolation.

So, now you see where interpolation becomes important, because this is what we have already discussed. Then there are methods which are sort of devised based on finite differences. So, this we have also looked at it how and there are methods which are based on undetermined coefficients. So, these are the 3 ways one can find the numerical differentiation, let us start with the methods which are based on interpolation.

So, in that case, what happens let us say there is a given function $f(x)$ at a set of (n + 1) distinct tabular points as that $x_0, x_1, x_2, \dots x_n$. So, we can first write the interpolating polynomial $P_n(x)$, and then differentiate the $P_n(x)$ to r times, so we can do that r lies $1 \leq r \leq n$. So, to obtain, so once we do that so, we will get ${P_n}^r(x)$. So, the value of this at let us say point x^*, which may be a tabular point or a non-tabular point gives the approximate, so these will give approximate value of $f^r(x)$ at $x = x^*$.

So, we can use the Lagrange interpolating polynomial such that

$$P_n(x) = \sum_{i=0}^{n} l_i(x)\, f(x_i)$$

this is 1 and we can have the error term like

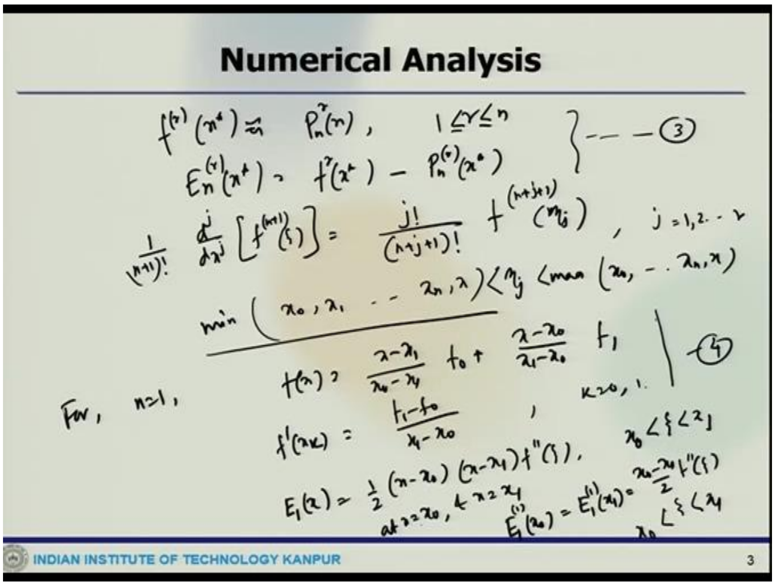
$$E_n(x) = f(x) - P_n(x)$$

which is one can write like

$$E_n(x) = \frac{(x - x_0)(x - x_1) \dots (x - x_n)}{(n + 1)!} f^{(n+1)}(\xi)$$

so this is equation 2.

(Refer Slide Time: 04:14)



So, what we can obtain is that

$$f^{r}(x^{*}) = {P_n}^{r}(x)$$

where $1 \le r \le n$ and we can get

$$ {E_n}^{r}(x) = f^{r}(x^{*}) - {P_n}^{r}(x^{*})$$

so, this is equation number 3. So, this is the error of the differentiation so, that is what we get. Now, the error term in equation 3 can be obtained by using formulas such that like

$$\frac{1}{(n+1)!}\frac{d^j}{dx^j}\left[f^{(n+1)}(\xi)\right] = \frac{j!}{(n+j+1)!}f^{(n+j+1)}(\eta_j)$$

where j goes from 1, 2 to r.

And where the points like

$$\min(x_0, x_1, x_2, \dots x_n, x) < \eta_j < \max(x_0, x_1, x_2, \dots x_n, x)$$

so, this is what it lies. Now, in the tabular points are equispaced we may use Newton forward or backward difference formula for let us say n =1 one can get

$$f(x) = \frac{x - x_1}{x_0 - x_1}f_0 + \frac{x - x_0}{x_1 - x_0}f_1$$

and

$$f'(x_k) = \frac{f_1 - f_0}{x_1 - x_0}$$

where k goes from 0, 1 and so on.

And differentiating the expression for error interpolation, we get

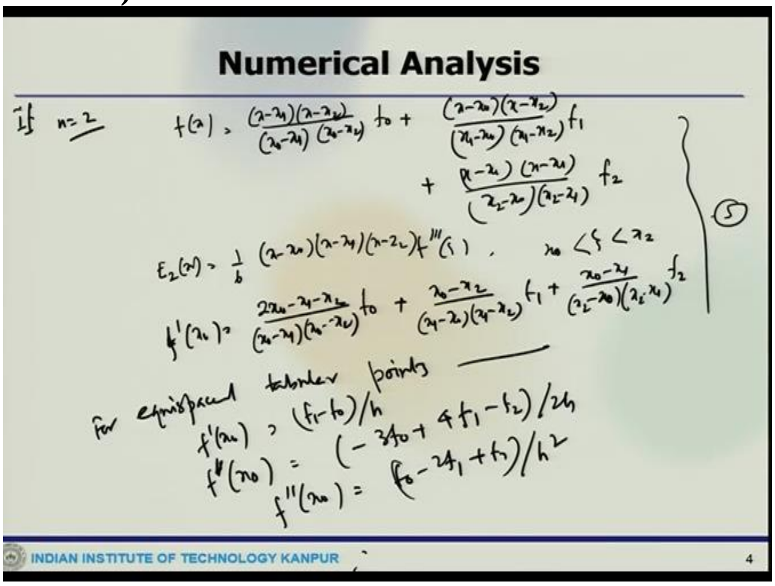
$$E_1(x) = \frac{1}{2}(x - x_0)(x - x_1)f''(\xi)$$

where $x_0 < \xi < x_1$. So, we get when at $x = x_0$ and $x = x_1$ what we can get is that

$$E_1^{(1)}(x_0) = E_1^{(1)}(x_1) = \frac{x_0 - x_1}{2} f''(\xi)$$

so this is what you get. So, these are set of equations for let us say equation 4 so, this is where $x_0 < \xi < x_1$.

(Refer Slide Time: 07:28)



Similarly, one can find out the error approximation for like the n = 2, so if n = 2 then what you finally get is that you get some similar way you can

$$f(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_2)} f_2$$

So, now, the error for that would be

$$E_1(x) = \frac{1}{6}(x - x_0)(x - x_1)(x - x_2) f'''(\xi)$$

where $x_0 < \xi < x_2$.

And similarly, you can find

$$f'(x_0) = \frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{x_0 - x_1}{(x_2 - x_0)(x_2 - x_2)} f_2$$

so, these are let us say equation 5. So, we can carry out the similar exercise and then finally, this is where the things are not, but finally if things are for equispaced tabular points things would become much simpler. So, this one can write that

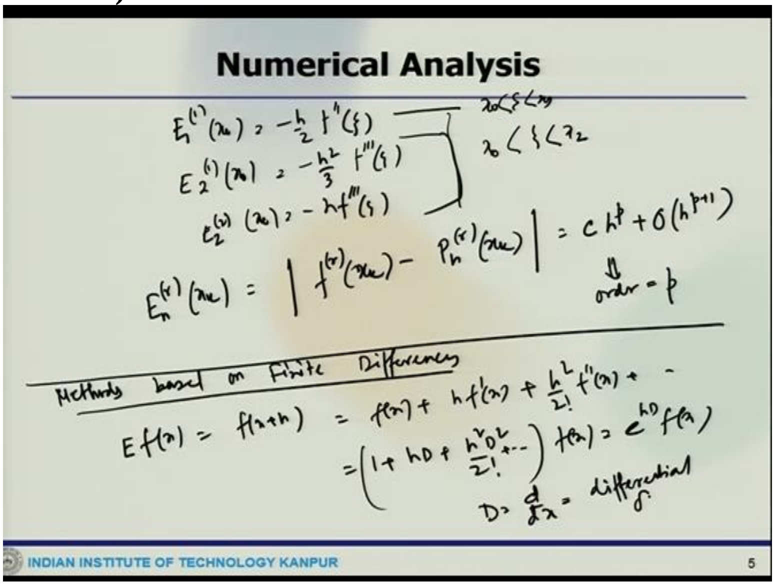
$$f'(x_0) = \frac{(f_1 - f_0)}{h}$$

$$f''(x_0) = \frac{(-3f_0 + 4f_1 - f_2)}{2h}$$

or

$$f''(x_0) = \frac{(f_0 - 2f_1 + f_2)}{h^2}$$

(Refer slide Time: 10:15)



And similarly, the error term would come along the way like this is for equispaced system where

$$E_1{}^{(1)}(x_0) = -\frac{h}{2}f''(\xi)$$

and then

$$E_2{}^{(1)}(x_0) = -\frac{h^2}{3}f'''(\xi)$$

And

$$E_2{}^{(2)}(x_0) = -hf'''(\xi)$$

so, all this where $x_0 < \xi < x_2$.

So, essentially you can write a generic expression of that

$$E_n{}^{(r)}(x_k) = \left|f^{(r)}(x_k) - P_n{}^{(r)}(x_k)\right| = ch^p + O(h^{p+1})$$

so C is a constant independent of h then the method is said to be order of so, here the order would be a p th order. So, you can see the one which for n = 1 that would be so, here what we wrote this is first order and this the other 2 written here this is second order.

So, we can determine the from this what would be the now, we look at some methods which is based on finite differences. So, here let us say consider relationship

$$Ef(x) = f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \cdots$$

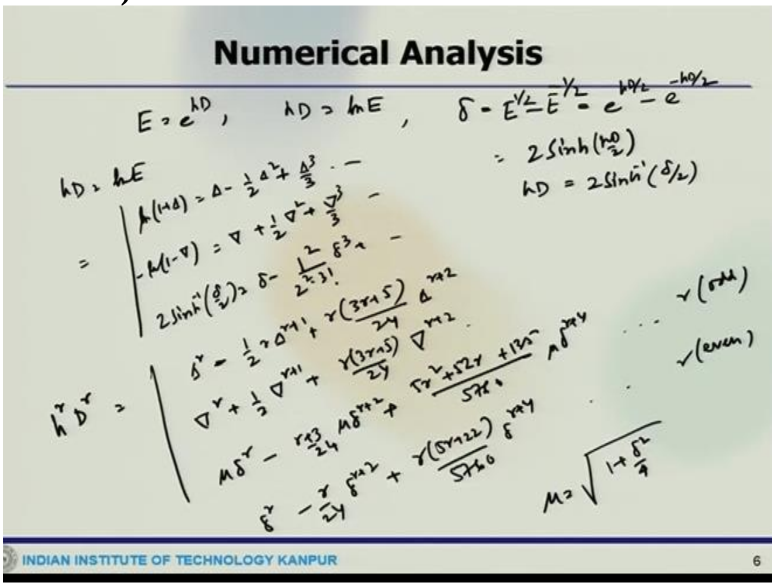
$$= \left(1 + hD + \frac{h^2}{2!}D^2 + \cdots\right)f(x) = e^{hD}f(x)$$

Or

$$D = \frac{d}{dx}$$

so, difference operators, so, this is called differential operators.

(Refer Slide Time: 12:50)



Now, symbolically what we can write that

$$E = e^{hD}$$

or

$$hD = \ln E$$

and we have

$$\delta = E^{\frac{1}{2}} - E^{-\frac{1}{2}} = e^{\frac{hD}{2}} - e^{-\frac{hD}{2}} = 2\sinh\left(\frac{hD}{2}\right)$$

Hence

$$hD = 2sin^{-1}(\delta/2)$$

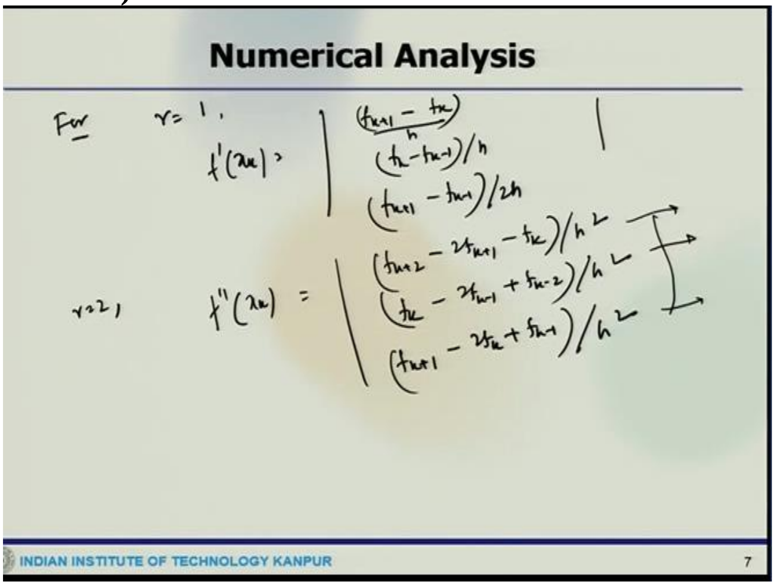
Now we have $hD = \ln E$. So, what we can write?

So, where

$$\mu = \sqrt{1 + \frac{\delta^2}{4}}$$

is the averaging operator and this is used to avoid offset of steep points in the method. Now, retaining various order differences in these equations here, which is shown here, we obtained different order methods for a given value of r.

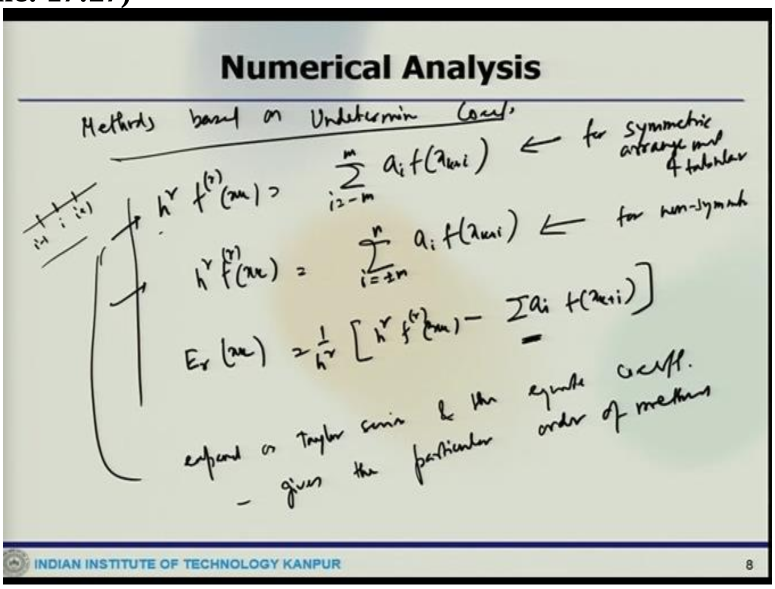
(Refer Slide Time: 16:05)



Like for let us say for if we get so, if we see this this is what how you can get a method which is based on this difference operator. And now, for different values of r let us say for r = 1 what do you get that $f'(x_k) and\ f''(x_k)$.

So, these are the different set of order of a system that you can get this is first order this is second order and this is forward this is backward and this is central. So, this is what the finite difference operator does and gets you different kinds of these things.

(Refer Slide Time: 17:27)



So, now, what we can look at is that methods which are based on undetermined coefficient so, here we write that

$$h^r f^{(r)}(x_k) = \sum_{i=-m}^{m} a_i f(x_{k+1})$$

for systematic arrangement of tabular points are what and let us say we write

$$h^r f^{(r)}(x_k) = \sum_{i=\pm m}^{m} a_i f(x_{k+1})$$

So, this is written for symmetric arrangement of tabular point that means.

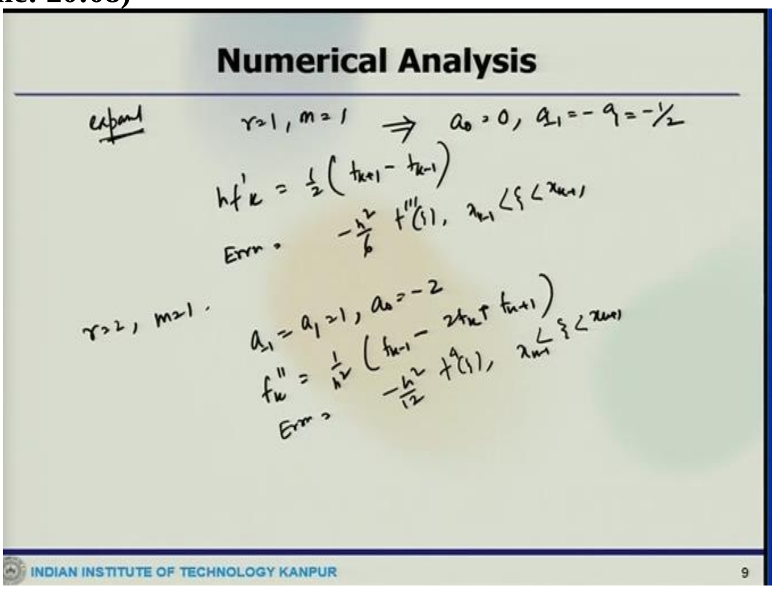
So, that things are not in a symmetric order and the error term would be defined as

$$E_r(x_k) = \frac{1}{h^r}\left[h^r f^{(r)}(x_k) - \sum a_i f(x_{k+1})\right]$$

So, this would be now the coefficient a_i here rather these all 3 sets of equations are determined here or here in this by recurring the method to be particular order. So, we expand each term in either of this equation or first one of the second one and the right hand side in Taylor series about the point x_k.

And then equating the coefficient various orders of derivative on both sides, here essentially you have to expand as Taylor series and then equate coefficient. So, that gives the particular order of the method. So, whether it could be the first order or second order whatever it is, it is going to come out to be like that.

(Refer Slide Time: 20:08)



So, now one can do all this like for example, one can expand these things and find out the coefficients for r = 1, m = 1 case, then you can find all coefficients which will come like $a_0 = 0$, $a_{-1} = -a_1 = -\frac{1}{2}$. So, where you get

$$hf_k' = \frac{1}{2}(f_{k+1} - f_{k-1})$$

or similarly, and the error term would be

$$Error = -\frac{h^2}{6}f'''(\xi)$$

for $x_{k-1} < \xi < x_{k+1}$.

Similarly, you can expand r = 2, m = 1 and you will get all these terms like

$$a_{-1} = a_1 = 1, a_0 = -2$$

So, where are you get

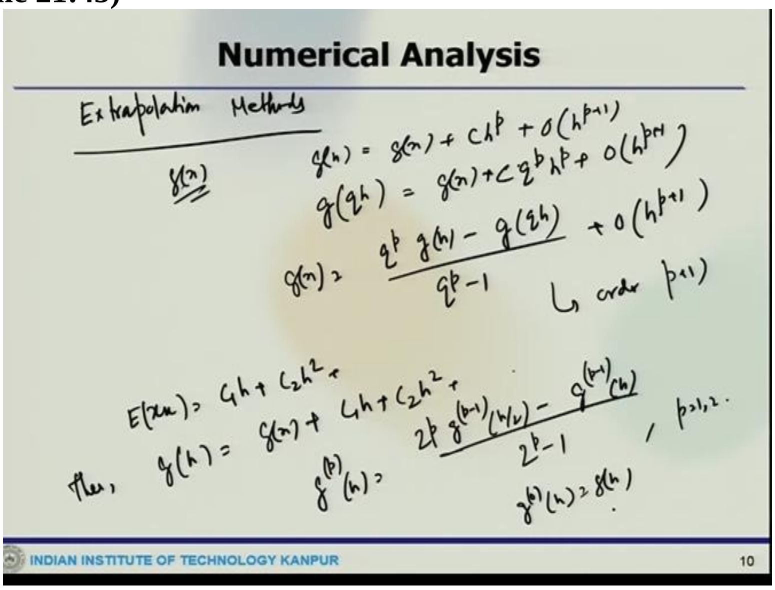
$$f_k'' = \frac{1}{h^2}(f_{k-1} - 2f_k + f_{k+1})$$

So, where the error would be

$$Error = -\frac{h^2}{12}f''''(\xi)$$

where $x_{k-1} < \xi < x_{k+1}$, so, these are second order system one can see that and one can find for m = 2 also for this thing.

(Refer Slide Time 21:45)



Now, there is another way one can look at is that some sort of an extrapolation method so, obtain accurate result, we need to use higher order methods which require a large number of function evaluations and may cause growth of round off errors. So, it is generally possible to optimum higher order solution by combining the computed values obtaining by using a certain lower order method with finite state.

Let us say for example, $g(x)$ denoted a quantity

$$g(h) = g(x) + Ch^p + O(h^{p+1})$$

or

$$g(qh) = \ g(x) + Cq^p h^p + O(h^{p+1})$$

So, from here once we eliminate C what we get

$$g(x) = \frac{q^p g(h) - g(qh)}{q^p - 1} + \ O(h^{p+1})$$

So, this defines a method of order (p + 1) order, so this order would be (p + 1) order, so this is called, this procedure is called the extrapolation or Richardson extrapolation, if the error term of the method can be written as a power series is h then repeating this extrapolation term, so, what we can write for the error you can write

$$E(x_k) = C_1 h + C_1 h^2 + \cdots$$

then we have

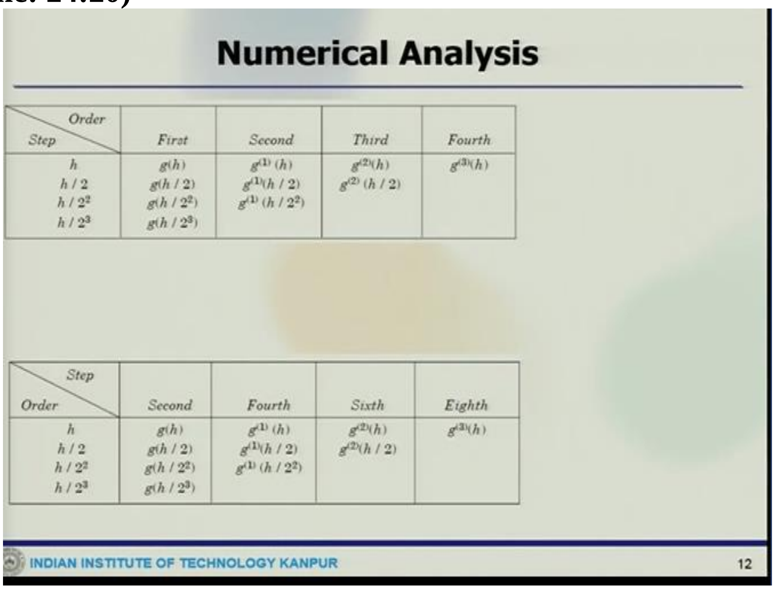
$$g(h) = g(x) + C_1 h + C_1 h^2 + \cdots$$

So, essentially one can write

$$g^p(h) = \frac{2pg^{(p-1)}(h/2) - g^{(p-1)}(h)}{2^p - 1}$$

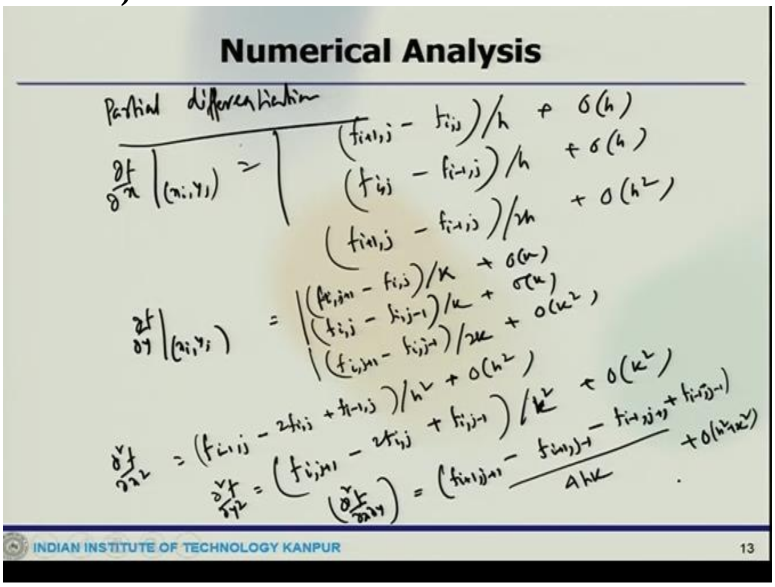
where p goes from 1, 2 so on and $g^0(h) = g(h)$.

(Refer Slide Time: 24:20)



So, then one can find the extrapolation table so, like you can see this is what the extrapolation table what so, this is the order of the system, so, this will be order this is the step. So, this is first order, second order, third order or fourth order and this is what the stepwise similarly, how you get these things, so, this gives you an idea about how to write all these.

(Refer Slide Time: 24:48)



Now, we can write also partial differentiation like for example, we can write

$$\frac{\partial f}{\partial x}_{(x_i, y_i)}$$

Which we can write as shown on the screen.

Similarly, one can write

$$\frac{\partial f}{\partial y}_{(x_i, y_i)}$$

similarly, one can write the second derivative like

$$\frac{\partial^2 f}{\partial x^2}$$

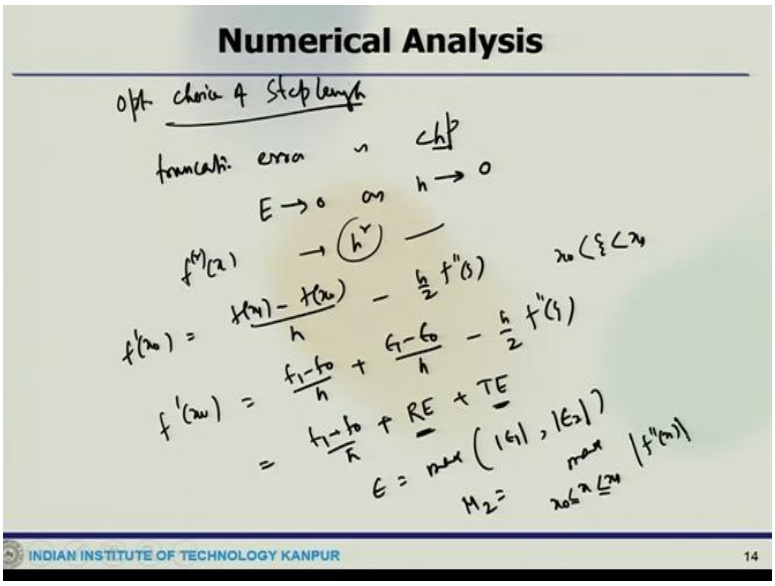
or

$$\frac{\partial^2 f}{\partial y^2}$$

And

$$\frac{\partial^2 f}{\partial x \partial y}$$

(Refer Slide Time: 27:42)



So, this is another one which you can have now the thing which one can have also optimum choice of step length like any numerical differentiation method, the area of approximation or the truncation error is of the form of Ch^p. Now, which should be tends to 0 so, this error should tend to 0 and h tends to 0. However, the method which approximates $f^r(x)$ contents h^r in the denominator.

So, h is successively decreased to small values, the truncation error also decreases, but the round off error in that method may increase when we are dividing by the smaller number so, in this case truncation error decreases, but the round off error may increase. So, the errors should be always within the limit and one so to see the effect of the sound of error in a numerical difference in method.

Let us consider

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{h} - \frac{h}{2} f''(\xi)$$

where $x_0 < \xi < x_1$. So, which you can write

$$f'(x_0) = RE + TE$$

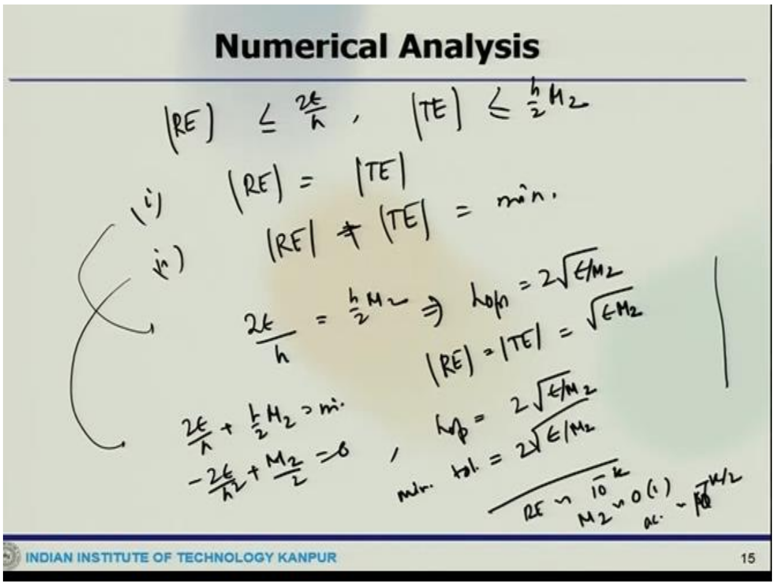
Now, round off error plus truncation error this is round off error truncation error. So,

$$\epsilon = max(|\epsilon_1|, |\epsilon_2|)$$

And

$$M_2 = \max_{x_0 \le x \le x_1} |f''(x)|$$

(Refer Slide Time: 29:55)



So, the round off error magnitude should be

$$|RE| \leq \frac{2\epsilon}{h}$$

and

$$|TE| \leq \frac{h}{2}M_2$$

So, we may call that a value h an optimum value of which one the following criteria is satisfied. So, one is that round off error would be truncation error or round off error plus truncation error is minimum. So, now, if we use the first criteria here, then what we get

$$\frac{2\epsilon}{h} = \frac{h}{2}M_2$$

So, from here we get

$$h_{opt} = 2\sqrt{\epsilon/M_2}$$

and round off error and truncation error they would be

$$|RE| = |TE| = \sqrt{\epsilon M_2}$$

So, now, if we use the second criteria, then this would be

$$\frac{2\epsilon}{h} + \frac{h}{2}M_2 = min$$

which gives

$$-\frac{2\epsilon}{h^2} + \frac{M_2}{2} = 0$$

where this is we get

$$h_{opt} = 2\sqrt{\epsilon/M_2}$$

So, the minimum tolerance is

$$Max. Tol. = 2\sqrt{\epsilon/M_2}$$

so, this is what we get. So, now this means that if the round of error is order of 10^{-k}, then $M_2 \sim O(1)$, then the accuracy given by the method may be approximately the order of accuracy would be order of sort of

$$ac. \sim 10^{-k/2}$$

So, this is how one can find out the optimum step size, what should be taken into consideration. So, that is what we wanted to talk about on differentiation, stop it here and continue the integration in the next session.