Computational Science in Engineering
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Lecture – 26
Numerical Analysis

So, let us continue the discussion on this error and other numerical methods. So, we have looked at how the round off error and all these, they arise now we will look at the truncation error.

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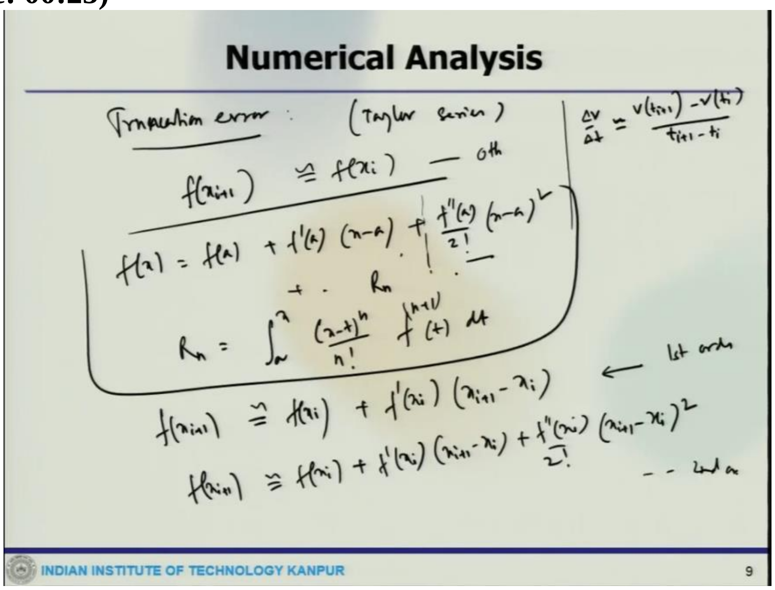

And this will arrive when we approximate a function using Taylor series approximation. So, let us say you have a function you try to show this will appear in Taylor series approximation, let us see you have I mean simple way to look at that if you try to look at $f(x_{i+1})$. Now what Taylor's theorem say that any function at $f(x)$, we can define

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots$$

Now I mean after some point of time we can say this is the term which is called remainder and the remainder would be

$$R_n = \int_a^x \frac{(x-t)^n}{n!} f^{(n+1)}(t)\, dt$$

So, wherever we stop it if we stop it here then this would be the remainder in the Taylor series approximation. Now one then this is for the Taylor series one actually expands the Taylor series. Now the thing which can happen is that this one way we have seen that 0th order approximation would be like this. Now if we use the Taylor series this guy can be actually approximated in a different way which is let us say we take another term which is

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

So, we are considering one more Taylor series, so that we have this approximation that is one can write. Now that will go from 0th order to another order but still if you see here, so we are considering this particular term but from here we have already omitted out some of the term which could lead to the error. So, this is still if this one is 0th order, this is first order or one can write like that considering one more term which is going to be like

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

And

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

So, this is second order, so this is the way you can keep increasing the number of points and your order could be increased. And finally, one can consider multiple number of points. And finally let us say if I go like that.

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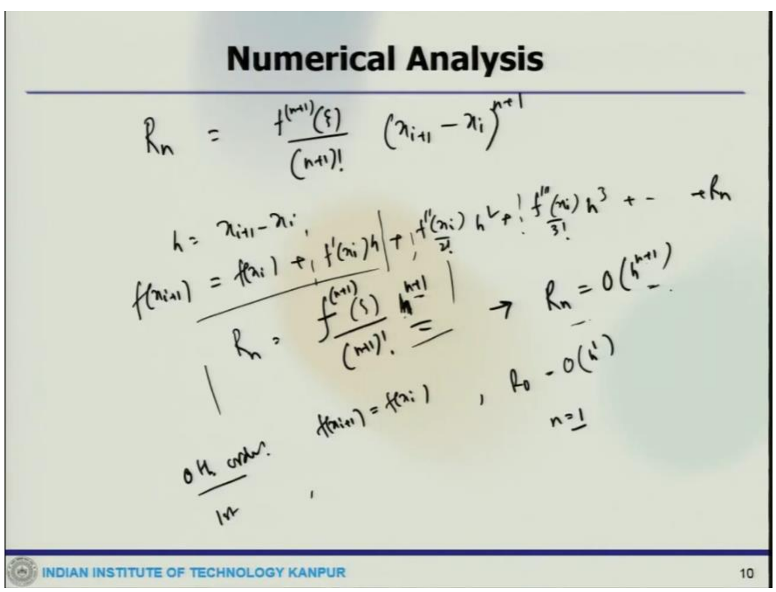

Then I can still write the remainder like

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x_{i+1} - x_i)^{n+1}$$

Now here n is the connect this is the remainder of the nth order approximation. For example, if you see when the first order approximation then we have omitted term from here. So, n would be 2, second order approximation we have left out the term from the third order. So, this n defines the order of approximation that is there.

Now if your step size is let us say $h = x_{i+1} - x_i$ then one can write

$$f(x_{i+1}) \cong f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{2!}h^3 + \cdots + R_n$$

So, essentially the R_n, we can write like

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}$$

So, we can have that is in the based on the step size. Now whatever would be the term remaining in the remainder that will determine that what the order of approximation that we have taken.

So, essentially if you look at this is order of h^{n+1}. So that means anything you are leaving out from this approximation that would be the order of a truncation error and this is where the truncation error may appear if you are leaving out on from here or if you are leaving out term from here. So that would lead to the kind of error which may be the problematic in your numerical approximation.

Now I mean one can see if you can just to extend this if you do the 0th order approximation which is $f(x_{i+1}) \cong f(x_i)$ then your order is so the remainder will be order of h and this would be that so, you have left out the term from here, so this would be the n is 0. So, that is what h is 1 so that means it is 0th order approximation so depending on the n you get the order. So, now if it is first order then n would be actually 1. So, you take up to this, so then accordingly your remainder would be the system. Now so these things are also important because one has to look at that.

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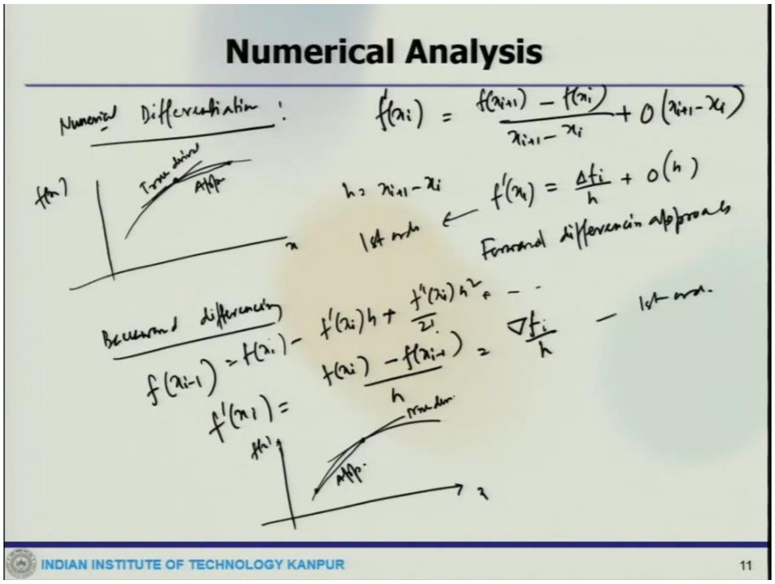

Now the other thing which would come is the numerical like the differentiation, so numerical differentiation, so which is like we are writing

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

So, this again comes from the Taylor series approximation if you see this, so this is the term we are trying to approximate. So, here we are writing because our h is $x_{i+1} - x_i$ that step size

So, this is essentially in writing effects in

$$f'^{(x_i)} = \frac{\Delta f_i}{h} + Oh$$

So, this is called forward differencing approach and this approximation particularly this is this first order. So, now we can have also second order forward differencing or second order approximation. So, the thing was to be, now similarly one can have backward differencing. So, you can look at the backward differencing also like for example will define the Taylor series for $f(x_{i-1})$.

Which is kind of

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

So, in the backward differencing where do we write that this would be written as

$$f'^{(x_i)} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{\nabla f_i}{h}$$

so this is called the first order backward differencing approach which is like you can see this one even in the graphically like if you have a $f(x)$ and this is x and this is how the function going on.

And this is the tangent that is a true derivative. Then from here the approximation going here, so this is the approximation. Now this case one can see this is the function you have the function in like this. So, this is the true derivative and from here this is for the approximation. So, this goes in a backward fashion. So, the important point to note here is that whether it is a forward or backward everything actually comes from the Taylor’s series expression.

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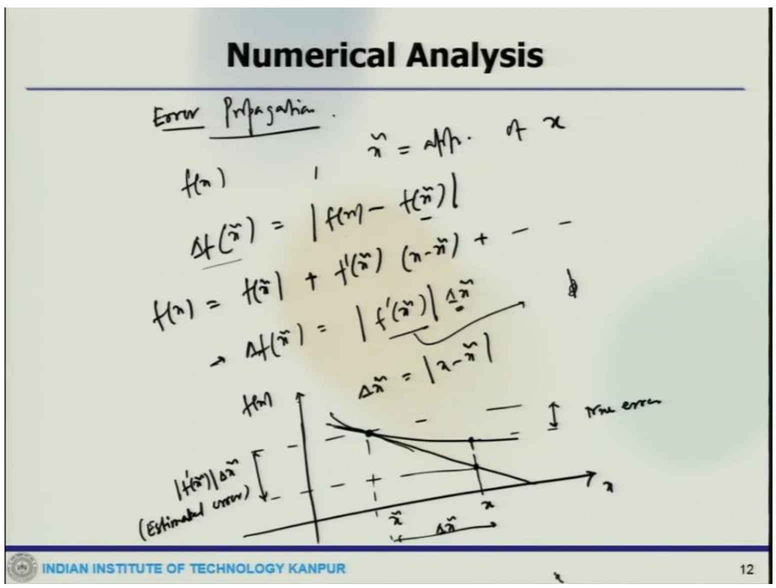

Now another thing which one can note that see we are talking about this error, so now the error propagation. So, either can propagate weather in the positive direction or negative direction. Suppose let us say we have a function $f(x)$ that is dependent on single variable x. And assuming that $\tilde{x}$ is an approximation of x. Now we would like to assess the effect of the discrepancy between x and $\tilde{x}$ on the value of the function.

So, let us say we would estimate $\tilde{x}$ is

$$\tilde{x} = |f(x) - f(\tilde{x})|$$

now here the evaluating this the problem here in evaluating these guys the value of $f(x)$ which is unknown. So, how we can overcome this? So, we can actually overcome by using the Taylor series approximation and through this approximate value, so what do you write

$$f(x) = f(\tilde{x}) + f'(\tilde{x})(x - \tilde{x}) + \cdots$$

So, we can write now

$$\Delta f(\tilde{x}) = |f'(\tilde{x})|\Delta\tilde{x}$$

where this guy is essentially represents the difference, now and $\Delta\tilde{x}$ is represent the error which is $(x - \tilde{x})$ estimate the error of x. So, this particular expression provides the capability to approximate the error in $f(x)$ for a given derivative. And how one can see that graphically let us see if you have a function $f(x)$ and this is going on x and this is the curve.

Let us say this is the tangent and so this goes like this. So, this is our true error and this guy is the $|f'(\tilde{x})|\Delta\tilde{x}$ which is sort of an estimated error and this would be our this is $\Delta\tilde{x}$ this is x, so these differences $\Delta\tilde{x}$. So, you can see what is true error what is estimated error and how we see these things.

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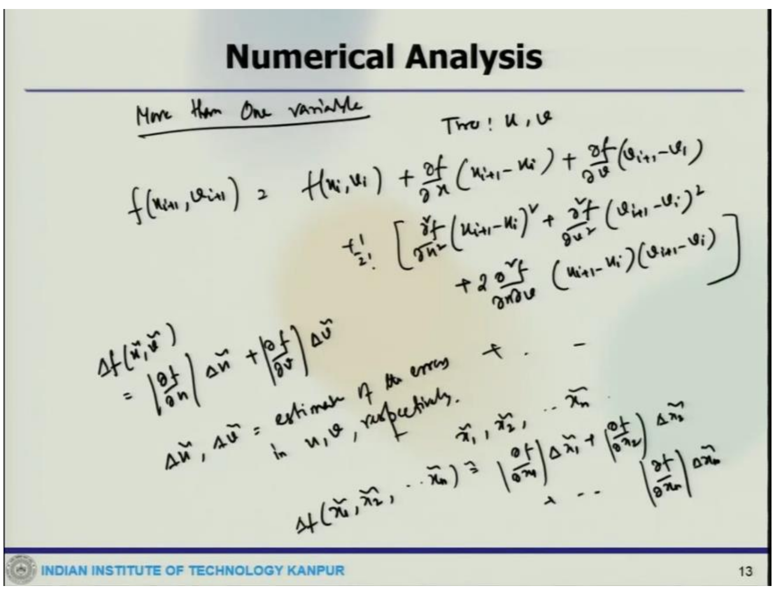

Now we can have also this thing for more than one variable like same Taylor series expression for more than one variable. So, we can generalize that let us say we have two independent variables which is u and v, then the Taylor series can be written as

$$f(u_{i+1}, v_{i+1}) = f(u_i, v_i) + \frac{\partial f}{\partial u}(u_{i+1} - u_i) + \frac{\partial f}{\partial v}(v_{i+1} - v_i)$$
$$+ \frac{1}{2!}\left[\frac{\partial^2 f}{\partial u^2}(u_{i+1} - u_i)^2 + \frac{\partial^2 f}{\partial v^2}(v_{i+1} - v_i)^2 + 2\frac{\partial^2 f}{\partial u \partial v}(u_{i+1} - u_i)(v_{i+1} - v_i)\right]$$

So, these are the term which will appear like this there will be so on. So, if you have now if all derivatives are evaluated the base point i and if all second order and higher order terms can be drop, then we can write that

$$\Delta f(\tilde{u}, \tilde{v}) = \left|\frac{\partial f}{\partial u}\right| \Delta\tilde{u} + \left|\frac{\partial f}{\partial v}\right| \Delta\tilde{v}$$

So, here $\Delta\tilde{u}$, $\Delta\tilde{v}$ these are the estimates of the errors in u and v respectively. So, we can see that now similarly if you have independent variables.

For example, $\tilde{x}_1, \tilde{x}_2, \tilde{x}_3, \dots, \tilde{x}_n$ then we can write that

$$\Delta f(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3, \dots, \tilde{x}_n) = \left|\frac{\partial f}{\partial \tilde{x}_1}\right| \Delta\tilde{x}_1 + \left|\frac{\partial f}{\partial \tilde{x}_2}\right| \Delta\tilde{x}_2 + \dots + \left|\frac{\partial f}{\partial \tilde{x}_n}\right| \Delta\tilde{x}_n$$

So, the one which we have looked at we can actually $\tilde{x}_n$ that concept to the higher level or more than one variable.

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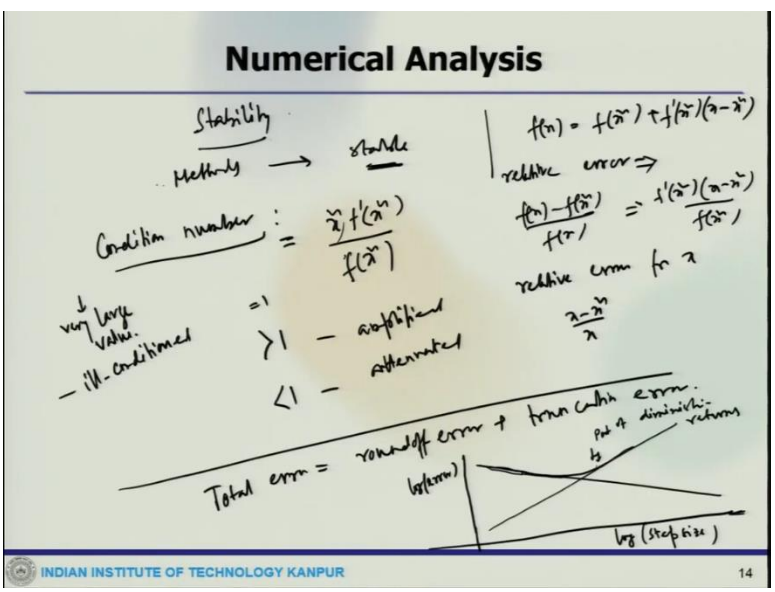

Now when we are talking about the error expression approximation then there is another thing would you talk about is the stability. So, now there is stability one is important because any of these numerical methods. The condition of a mathematical problem relates to its sensitivity to the change in its input values. So, we can say if the numerical results or numerical system is unstable if the uncertainty of the input values is grossly magnified by the numerical method.

So, that means the methods should be always stable that means it should be able to handle some of the uncertainties. Now one can we can look at this simply by looking at the Taylor series like what we had

$$f(x) = f(\tilde{x}) + f'(\tilde{x})(x - \tilde{x})$$

So, the relative error for $f(x)$ would be the relative error that we can estimate is that

$$\frac{f(x) - f(\tilde{x})}{f(x)} = \frac{f'(\tilde{x})(x - \tilde{x})}{f(\tilde{x})}$$

So, these are the errors that you have, so one important number which we will call the condition number. So, this can be defined as the ratio of these relative errors that means condition number is

$$\frac{\tilde{x} f'(\tilde{x})}{f(\tilde{x})}$$

So, this provides and measure of the extent to which an uncertainty in x range is magnified by $f(x)$. So, this will give you an idea like how the uncertainty in x or the input value can be magnified.

So, the value of one tells us that the functionality is identical to the relative error in x, a value greater than 1 tells us that the see if this is greater than 1 that means the error is amplified. If it is less than 1 that means the error or these things are kind of attenuated and equals to 1 means it tells us the functions relative error is identical to the relative error of the x. So, depending on this condition number.

Now so if sometimes if you have very large value of this condition number very large value, then this called the ill condition system and probably this ill condition system may not be a good idea or a good one to numerically handle. Now when you look at the total error, so you have total numerical error, so the total error would be sum of round of error plus truncation error and they are kind of depends on particularly stiff size.

Like if you have look at graphically if this is log of step size that is which is our h here difference or here if you see log of error. Now once the step size is increases in the log sense the log error also will increases like this the round off error also goes off. If step size is small, I mean this error would be small, step size is large this would be large so that total error could be the sum of this I mean like this, it goes in this kind of fashion. So, this is a point where point of sort of point of diminishing return. So, you can see how they are basically going to contribute to the system.

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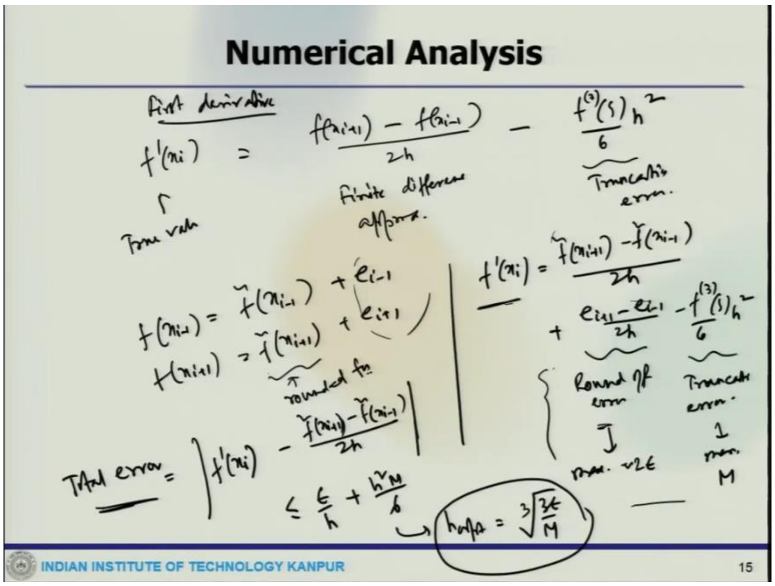

Now the numerical differentiation that we have looked at so we can see the error like for example we can talk about the first derivative and where we have

$$f'^{(x_i)} = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{f^3(\xi)}{6}h^2$$

So, this is my truncation error, so when I write the first derivative so if two function values in the numerator of the finite difference premise have no round off error then the error only is due to the truncation.

But we are using digital computer to solve this. So, the function values do include round off errors as like

$$f(x_{i-1}) = \tilde{f}(x_{i-1}) + e_{i-1}$$

error in that and

$$f(x_{i+1}) = \tilde{f}(x_{i+1}) + e_{i+1}$$

So, these are these guys are rounded function. So, one can say rounded function, so and e's are the associated round off error. Now once you substitute these things in this first derivative what we write

$$f'(x_i) = \frac{\tilde{f}(x_{i+1}) - \tilde{f}(x_{i-1})}{2h} + \frac{e_{i+1} - e_{i-1}}{2h} - \frac{f^3(\xi)}{6} h^2$$

So, this is again true value this is finite difference approximation. This is our round off error this is our truncation error. Now you can see when you do the approximation of the first derivative you get some truncation error you get some round off error. So, if they are ideally zero you get the proper approximation but in any numerical methods or any numerical methods when you transplant to the computer programming these are not going to be completely eliminated.

So, there but the way one has to handle that. So, now assuming that the absolute value of each component of the round off error has an upper bound of epsilon and the maximum possible value of the differences will be 2ϵ. So, this the maximum possible value is roughly 2ϵ then also the derivative that the third derivative has a maximum absolute value of M. So, this is having a maximum value of M.

Then we can write this total error which is

$$\left| f'(x_i) - \frac{\tilde{f}(x_{i+1}) - \tilde{f}(x_{i-1})}{2h} \right| \leq \frac{\epsilon}{h} + \frac{h^2 M}{6}$$

so that you can see that an optimal step size can be determined by differentiating this particular error. So, if you differentiate this error for the maximum for step size minimum or optimal step size the result gives us that.

So, if you do that from here one can get

$$h_{opt} = \sqrt[3]{\frac{3\epsilon}{M}}$$

So, this is the optimum step size that means all this error in this numerical approximation of first derivative I mean this is true for even higher order derivative like one can estimate second derivative one can estimate third derivative also. So, these are associated with this kind of round off error and now one has to when you devise a numerical method.

Obviously, these errors need to be controlled. So, unless you have, I mean either ideally you should have 0 of this rounds off error and truncation error which will lead to close or exact approximation but if not, one has to have a numeral algorithm in place or method in place. So that should lead to kind of reduce this error.

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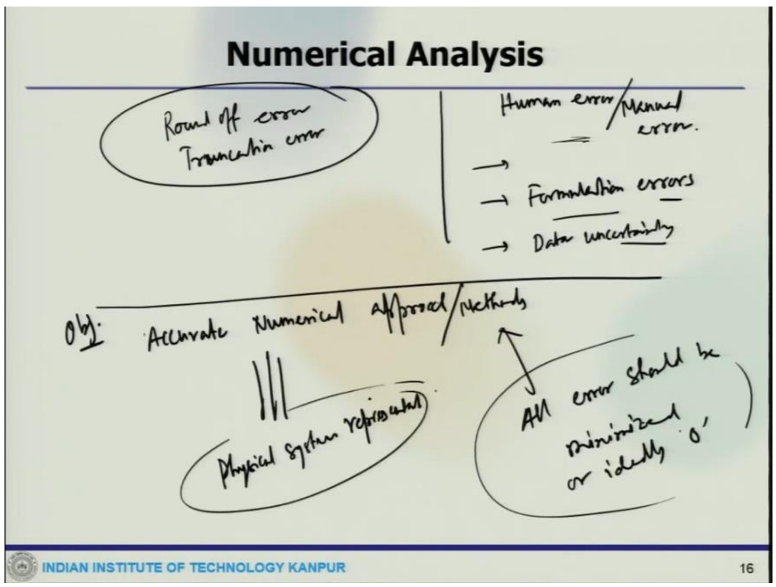

Now apart from this so you got all this round off error, truncation error these are what you can control through the numerical approach what is the optimal grip size and all these but there are some other things which can come from the human error or manual error like these are one can do a lot of blunders doing that. So, this can possibly happen during doing the mathematical modeling process, so can contribute to all other components of error.

So, if you have some sort of human error in some stage of this approximation this can lead to other errors or the total error. So, this would usually happen when then there could be another problem which could happen is that formulation error like when we are devising that approximate approach or the mathematical expression that time one can wrongly divide or formulate the system so that it can lead to the formulation error.

So, there is a possibility of that or one can have like data uncertainty. So that is another thing which can lead to some sort of an error also. So, in totality that one has to have an accurate so that is the objective rather accurate numeric or methods to have that you should have all errors should be minimized or ideally zero. So, if that is the case then any numerical approach which will be equivalent to our physical system representation.

Otherwise, it will represent a different physical system or different system of equation. So, whatever approximation we do. So, this is what one has to keep in mind when talking about numerical methods and these are sort of the background of it. Now we will continue our actual discussion in the next session.