Numerical Analysis
Prof. S. Baskar
Department of Mathematics
Indian Institute of Technology, Bombay

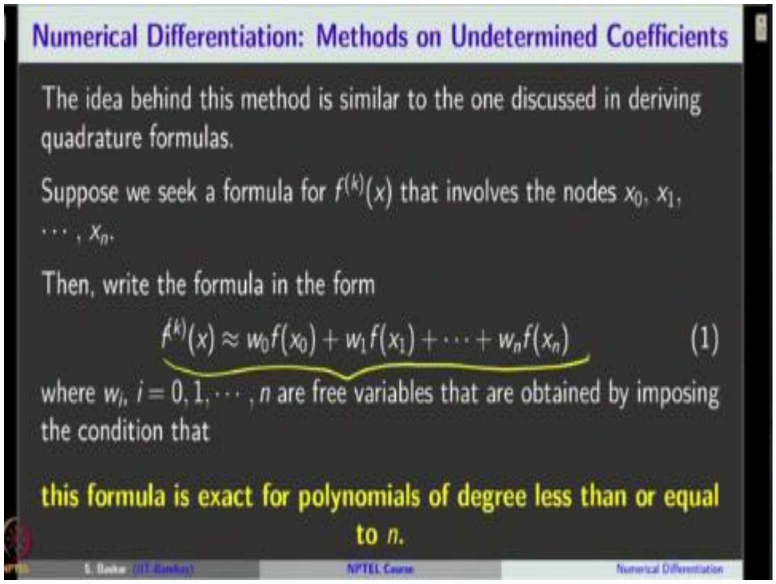
Lecture - 54
Numerical Differentiation: Method of Undetermined Coefficients and Arithmetic Error

Hi, we are deriving some finite difference formulas for approximating derivative of a given function. In the last class we have derived three primitive finite difference formulas for approximating the first derivative of a given function. Well, we started with the basic idea of getting these primitive formulas directly from the definition of the first derivative that we learned in the calculus course.

Then we also obtained these formulas through the interpolating polynomial of degree 1, for the function f and then we also extended this idea of using the interpolating polynomials to get finite difference formulas for derivatives of higher order. That is, you can also get the finite difference formula for f', f''' and so on. And also, you can get variety of finite difference formulas by choosing the degree of the interpolating polynomials.

And also, the positions of the nodes involved in the interpolating polynomials. In today's class we will have another way of deriving finite difference formulas. This is using the method of undetermined coefficients.

(Refer Slide Time: 01:45)



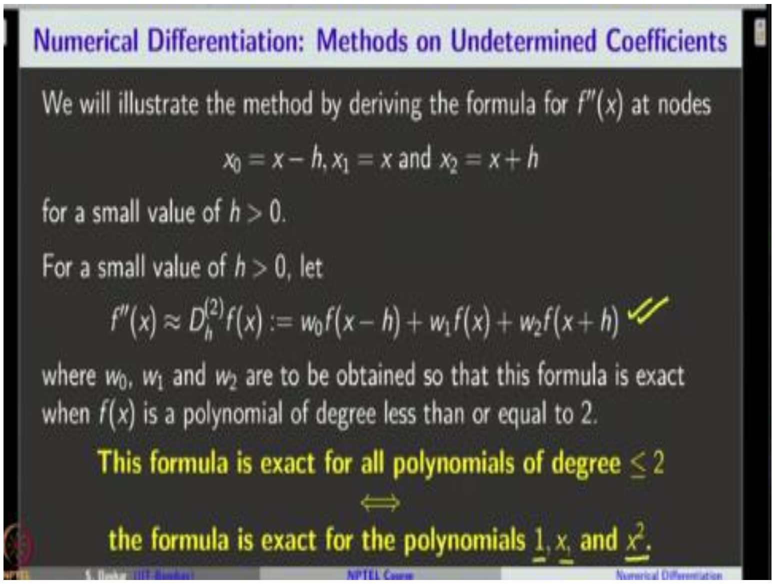
This method is not something new to us. We have already seen this idea, when we were deriving the quadrature formula for a given function. The idea is almost the similar. Let us see what is this idea? The idea behind the method of undetermined coefficients to derive certain finite difference formulas for a given function is the following. Suppose you want to derive a finite difference formula for the *k*th derivative of a function *f* at a point *x* involving the nodes $x_0, x_1, \cdots, x_n$.

Then what you do is, well basically you look for the finite difference formula in this form, that is $w_0 f(x_0) + w_1 f(x_1) + \cdots + w_n f(x_n)$. Here you already know what is $x_0, x_1, \cdots, x_n$ because these are given to us and we have to only find $w_0, w_1, \cdots, w_n$. Now how will you find? Well, you can find these unknown quantities by imposing the condition that this finite difference formula is exact, if the function *f* happens to be a polynomial of degree less than or equal to *n*.

What is this *n*? Well, that is the *n* that is chosen here, that is the number of nodes. If you are given *n* + 1 nodes, then you have to find *n* + 1 unknowns. These *n* + 1 unknowns therefore you have to impose the condition that this finite difference formula should be exact for polynomials of degree less than or equal to *n*. Why?

Because the space of all polynomials of degree less than or equal to *n* will have *n* + 1 basis elements. You take the monomial basis and then you can form a linear system with solution as the vector w, whose coordinates are $w_0, w_1, \cdots, w_n$. This is something which we have already done in the quadrature formula. The same idea goes through here also. Let us see how to go ahead with it.

(Refer Slide Time: 04:16)

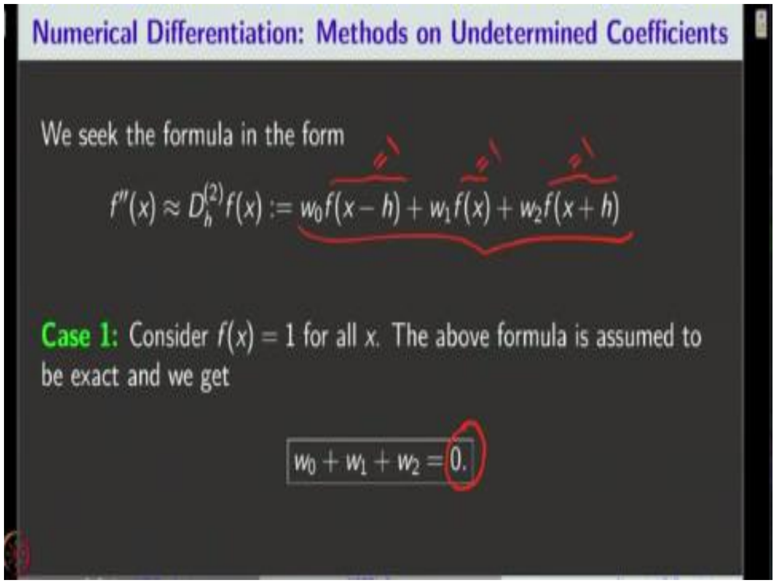


It is well understood through an example. Therefore, we will consider our nodes as $x_0 = x - h, x_1 = x$ and $x_2 = x + h$. That is, we are taking $n = 2$. If you recall, this is what we call as the central difference nodes and therefore the resulting finite difference formula will be called as the central difference formula. We will try to derive the formula for $f''(x)$. Well, what you have to do is, first write the general form of the finite difference formula by taking the central difference nodes.

And in order to get w_0, w_1 and w_2, you have to impose the condition that this central difference formula is exact for polynomials of degree less than or equal to 2. Which is equivalent to imposing the condition that this formula is exact for polynomials 1, x and x^2. Why we are restricting to only these particular polynomials? Because they form a basis for the space of all polynomials of degree less than or equal to 2.

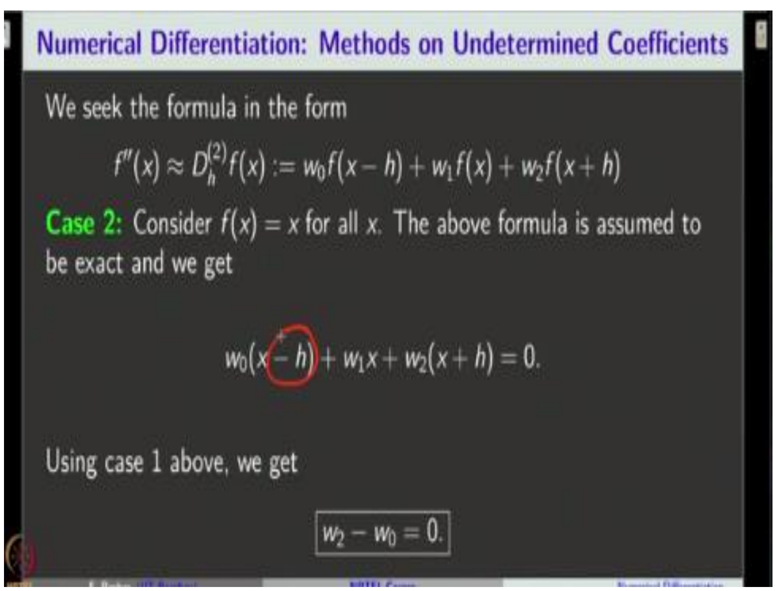
That is why we are restricting ourselves only to these particular polynomials which are polynomials of degree less than equal to 2. Now by considering each element of this basis we will get one linear equation in w_0, w_1 and w_2.

(Refer Slide Time: 05:58)



Let us do this, let us first consider the polynomial of degree 0, that is, let us consider the case when f = 1 for all x. In this case, as per our condition, this formula should give you the exact value for the $f''(x)$. What is $f''(x)$? If f happens to be the constant function, well that is 0. Therefore, you have $f''(x)$ = 0 and what is the expression coming from the finite difference formula? Well, you have to take f = 1. Here and that leads to $w_0 + w_1 + w_2$, therefore your first linear equation is given by this.

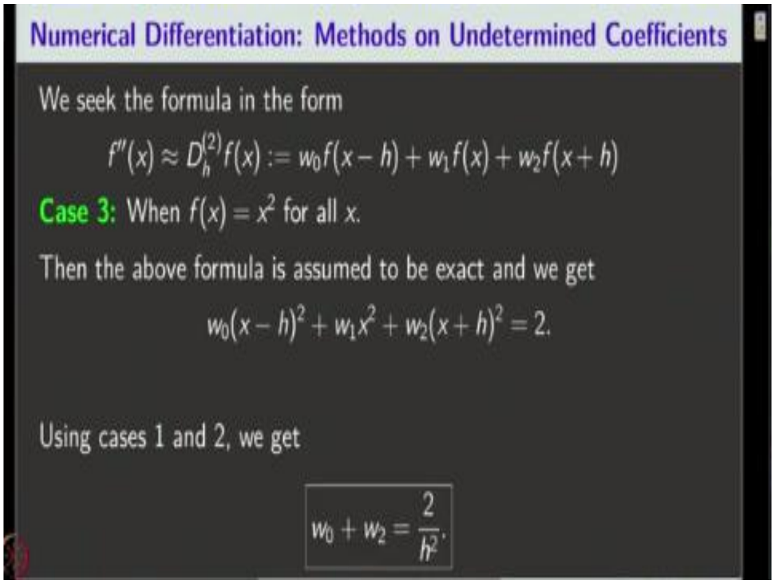
(Refer Slide Time: 06:57)



Let us go for the second case, that is, let us take $f(x) = x$. In this case again, $f''(x)$ = 0 and the right hand side will be given by $w_0(x-h)$ because $f(x) = x$, therefore you will have $w_0(x-h) + w_1 x + w_2(x+h) = 0$. And that is your second equation. Now what you do is, you can use the equation we have obtained in case one. What was that equation? It was precisely $w_0 + w_1 + w_2 = 0$.

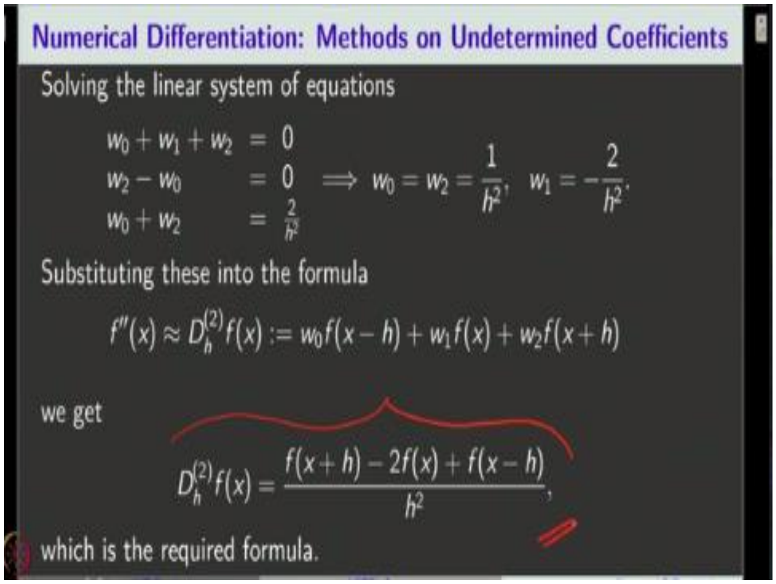
Therefore, these terms will disappear and you will be left out with $(w_2 - w_0)h = 0$, and we always assume that h is strictly greater than 0 therefore you will have $w_2 - w_0 = 0$ and that is the second equation.

(Refer Slide Time: 08:10)



Let us take the third case where $f(x) = x^2$ for all x. In this case, $f'' = 2$ and the right hand side expression will reduce to this, obviously again you can use the expressions that is the equations obtained in case 1 and case 2. And then you can reduce this equation to this equation.

(Refer Slide Time: 08:41)



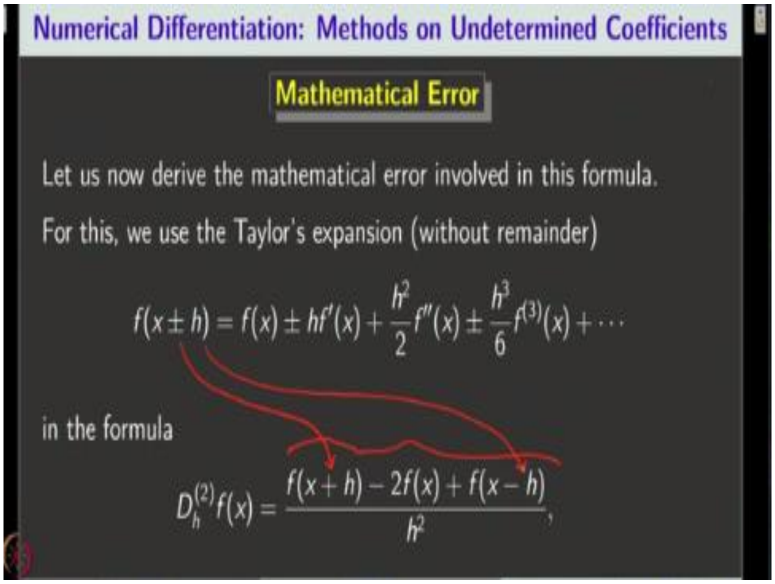
So, we got three equations by imposing three conditions and we have three unknowns w_0, w_1 and w_2 and they are appearing linearly in this system. Therefore, it is a linear system of equations. You can solve this system to get the values for w_0, w_1 and w_2 and those are given by these expressions. Now, what we have to do? Recall, that we have assumed that our central difference formula will look like this.

In this, these terms are known to us provided, of course, we know $f(x)$ and h then these three terms are known to us and now we also know w_0, w_1 and w_2. You just substitute these values into this expression. You can see that the central difference formula for approximating the second derivative of a function f at a point x is given by this formula. This is how we derive the central difference formula.

If you derive the central difference formula using the interpolating polynomial, you can see that that will also lead to the same expression. What you have to do is you have to take x_0, x_1 and x_2 as given here. This is the central difference nodes and then you write the Newton's form of interpolating polynomial using these nodes. That will be a quadratic polynomial, differentiate it twice and substitute x_0, x_1 and x_2 into it.

Then also, you will get the finite difference formula exactly the same as what you got using the method of undetermined coefficients. Once you understand this idea, you can also derive the finite difference formula for the second derivative using forward nodes, backward nodes. Similarly, you can do for third order derivative and so on. Just like how you can do with interpolating polynomials, you can also do with method of undetermined coefficients. You can obtain definite difference formula of any order with any given nodes.

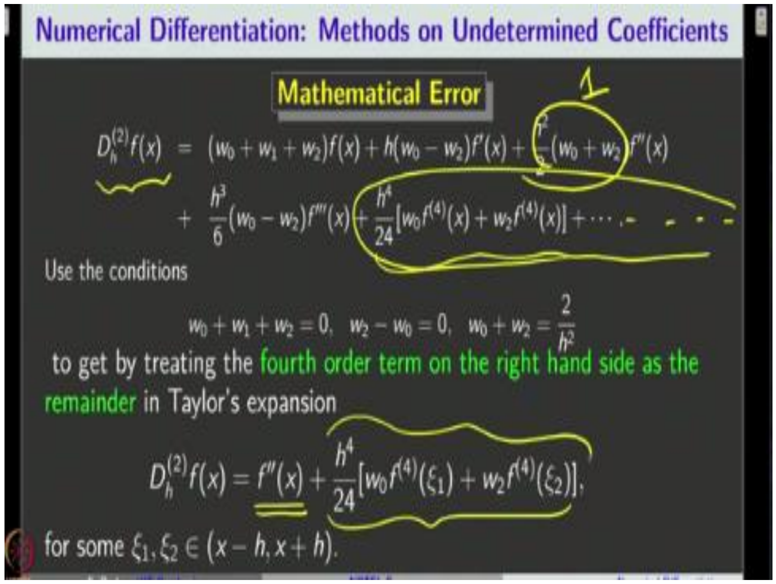
(Refer Slide Time: 11:11)



Let us try to derive the mathematical error involved in the central difference formula, that we have derived just now. For that again you have to use the Tylor's expansion. Remember, that the central different formula involves $f(x+h)$, therefore you have to use Taylor expansion for this term and also it involves $f(x-h)$. Therefore, you have to use Taylor's formula for this term also. That is why we are first writing the Taylor's formula for $f(x+h)$ as well as $f(x-h)$.

And remember the central difference formula is given like this, therefore you put the Taylor formula for $f(x+h)$ here. Similarly, the Taylor's formula for $f(x-h)$ here and try to simplify that expression.

(Refer Slide Time: 12:10)



If you substitute these two expansions, what you get is this expression for the central difference formula. You can see how you get it. You simply have to substitute this into this and then just group the similar terms. Then you will get this expression. Remember, I am not writing the Taylor's formula with the remainder, why because when you substitute this into this expression certain terms will get cancelled.

And therefore, at the beginning at this stage you do not know what will remain as the remainder term, that will come as the mathematical error finally in our expression. That is not very clear at present, therefore what I suggest you is, you write the Taylor's series. Substitute it into the expression, whatever may be the central difference formula you do. What you first do is, you write the Taylor's series and then substitute it into the finite difference formula.

And then group all the terms like this and see which are all the terms which are getting cancelled. In this case, if you see you got w_0, w_1 and w_2 in such a way that $w_0 + w_1 + w_2 = 0$. This is how you got the linear system for w. If you recall, we have just now seen that w_0, w_1 and w_2 satisfies a linear system. In that, the first equation is $w_0 + w_1 + w_2 = 0$. In fact, $w_0 - w_2$ is also equal to 0 and this is equal to $\frac{2}{h^2}$.

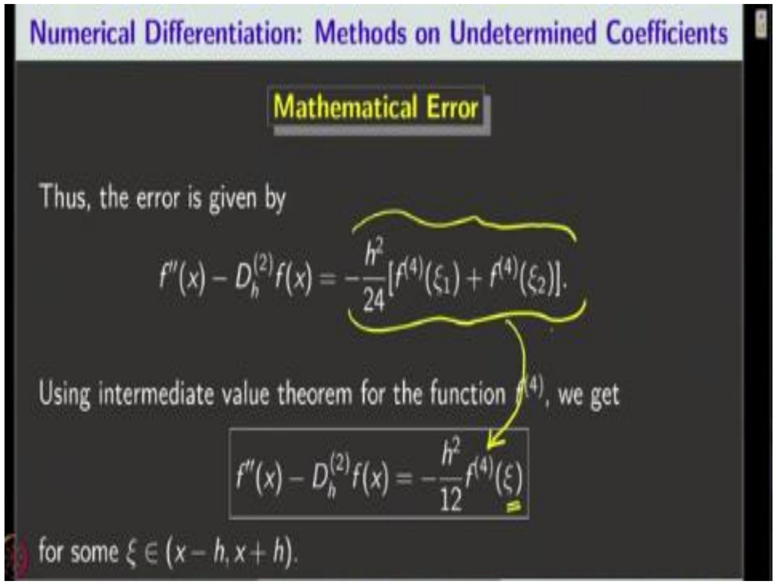
If you recall, that is what we obtained here. So, I am just using this in this expression and similarly this term is also going to 0, and what remains here is this term. So, this term onwards in this series will remain. Of course, certain terms may be 0 but the leading term remaining here is this term. Therefore, that gives us a clue that this term should be taken as the remainder and that will decide what is the order of accuracy of the central difference formula.

Let us see that your linear system was this, therefore by using this you can see that the fourth order term will survive in this expression because this goes off, this goes off and this goes off. This is going to contribute for your f''. You have $D_h^{(2)}, f''$ has to come to the other side in order to make it mathematical error and that will be equal to now this term. So, this gives us a clear idea of what you have to take as the remainder term.

This is very important while deriving the expression for the mathematical error. You do not decide something apriorly, because you may be writing the reminder term for this, but that is not correct because the term is very nicely getting off from your formula. And what actually dominates your error is this term. Therefore, this has to be taken as the remainder term. You have to keep this in mind very carefully.

And write finally that the left hand side, that is the central difference formula is equal to this term becomes 1 now. You have, therefore $f''(x)$, all other terms vanished and you are left out with this term plus something. But all that can be clubbed and made as the remainder term here which involves unknowns ξ_1 and ξ_2, where ξ_1 and ξ_2 are some unknown numbers lying between the nodes $x - h$ and $x + h$.

(Refer Slide Time: 16:39)

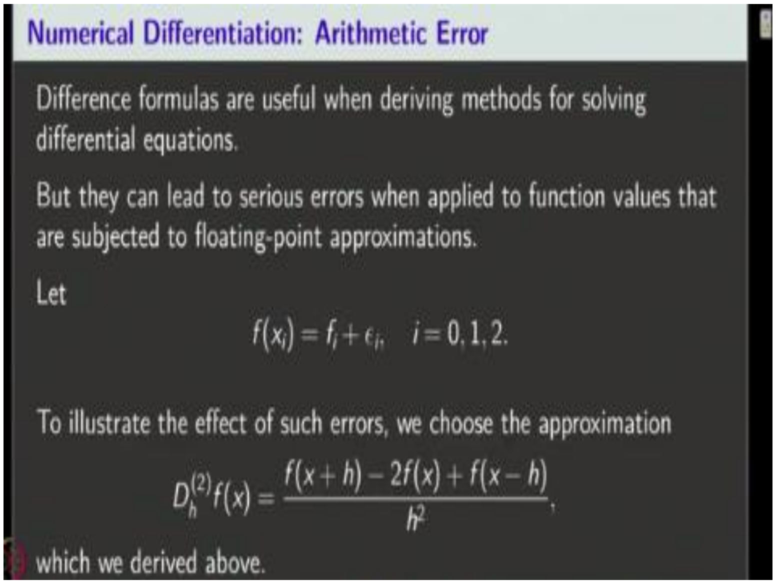


Now this is what finally we derived as the expression for the mathematical error. You see that this is the mathematical error and that is given by this, again you can use the intermediate value theorem. Recall, we have seen such a problem in one of our tutorial sessions, as I told in the last class. If you go to the lecture number 7, we discussed some tutorial problems in that lecture. In that you take the second problem.

You will get an idea of how to use the intermediate value theorem, in order to reduce this expression to this expression. I leave it to you to see that. By using that, you can in fact write this expression as $\frac{h^2}{12}$ into the fourth derivative of f for some unknown ξ lying between $x - h$ and $x + h$. So, finally this is the mathematical error for the central difference formula for $f''(x)$. Again, from here you can see what is the order of accuracy of this central difference formula for the second derivative of a function.

The order of accuracy is 2, that is it is the second order formula. This is all about how to derive a finite difference formula and how to obtain the mathematical error for that formula and also how to see what is the order of accuracy of that finite difference formula in approximating a derivative of some order of a function.

(Refer Slide Time: 18:54)



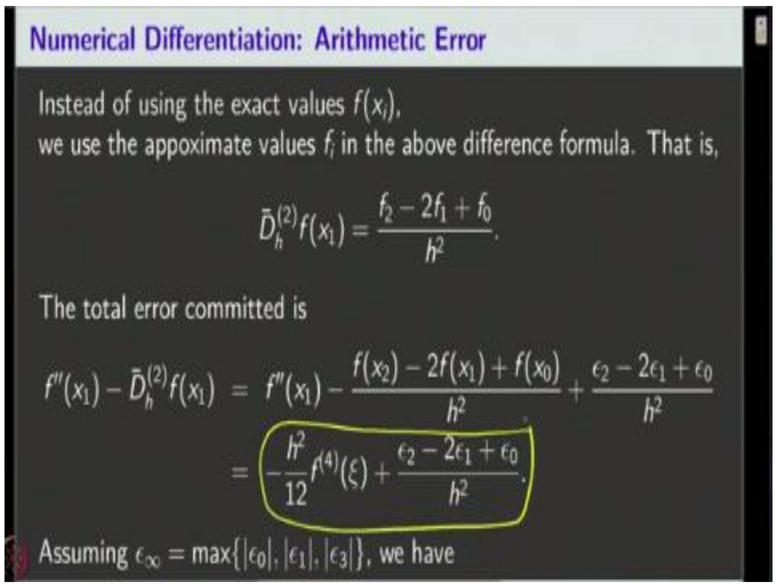
Now let us see how arithmetic error can be analysed in these formulas. In fact, the idea that I am going to introduce here for analysing the arithmetic error involved in finite difference formulas, can be used also to analyse the arithmetic error involved in quadrature formulas. Let us see how to analyse arithmetic errors in finite difference formulas. As you know finite difference formulas are useful in many practical applications. In particular, they are used in solving differential equations.

Similarly, quadrature formulas are also used in practical applications. They are very nice however they suffer very seriously from the arithmetic errors just like how the polynomial interpolation suffer. Similarly, the quadrature formulas and finite difference formulas will also suffer significantly due to arithmetic errors. These are quite expected because these formulas are derived basically from the polynomial interpolations. Therefore, they have to also suffer.

So, to analyse the arithmetic error involved in finite difference and quadrature formulas first what you do is, you write the exact value involved in the evaluation of the function at any point x_i, say is something like f_i, this is the approximate value. Just imagine that your computer evaluated the value of the function f at the point x_i and it gave this value to you. It obviously will involve certain rounding errors.

With that, it is supposed to give you this value but it gave you this value. And what is the error involved in it? We will denote that error by ϵ_i. So, since we are going to analyse the arithmetic error involved in the central difference formula with three central different nodes, I am just taking *i* to be 0, 1 and 2 that is we are going to have x_0, x_1 and x_2 as the nodes. And if you recall, if you take $x_0 = x - h, x_1 = x$ and $x_2 = x + h$, you will get the central difference formula in this form for approximating this second derivative of the function f at a point *x*. In this you are now involving an arithmetic error also.

(Refer Slide Time: 21:13)



Now let us see how this formula will look like if you use the approximate values instead of exact values of the function evaluated at the nodes. Then the central difference formula will look like this. I am using the approximate values of the function at the nodes. Let us denote the corresponding value by $\overline{D}_h^{(2)} f(x_1)$. Now our interest is to see, what is the total error involved in it, what is the total error.

Well, this is the exact value and this is the value given by your computer. Previously the mathematical error is the exact value minus the approximate value, that does not involve any rounding error. Now it is the approximate value that involves the approximation of the operator, that is the second order derivative operator as well as the approximation involving the rounding errors.

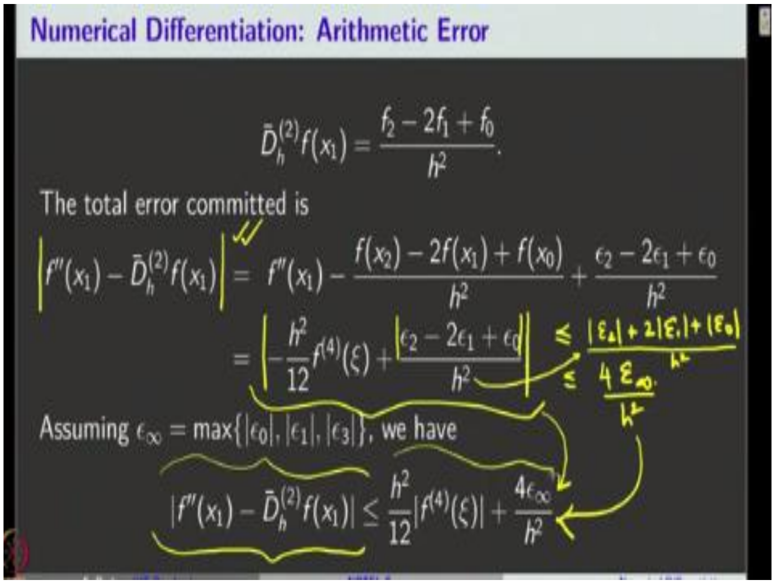
So, that is the total error and that is given by f$f'' - D_h^{(2)} f(x)$ and this is the mathematical error plus you can see that the arithmetic error now becomes like this. How will you get this? Simply what you have to do you have to subtract $D_h^{(2)} f(x_1)$ and add $D_h^{(2)} f(x_1)$. So that is what I am doing, f'' minus the exact operator is given like this. Then the exact operator minus the operator with rounding error will give you this expression.

Because the exact value minus the approximate value is taken as ϵ. That is why you will get I leave it to you to just derive this and see so, this is nothing but $D_h^{(2)} f(x_1) - \overline{D}_h^{(2)} f(x_1)$, that is what comes like this. You can easily derive that, so this step has to be done not only for the central difference.

If I ask you to derive the total error of any formula, any quadrature formula or any finite difference formula. What you have to do is, the total error then you add and subtract the formula without any arithmetic error and then you will get mathematical error plus the arithmetic error here. Now you know that the mathematical error expression for the central difference formula is given like this. Just now we have derived this expression for the mathematical error. And now we have the arithmetic error, just taken from here therefore this is the expression for the total error.

Just to have a clear idea of the behaviour of this expression, let us just take the maximum of all these ϵs and let us denote it by ϵ_∞. ϵ_∞ is the maximum of the absolute values of ϵ_0, ϵ_1 and ϵ_2.

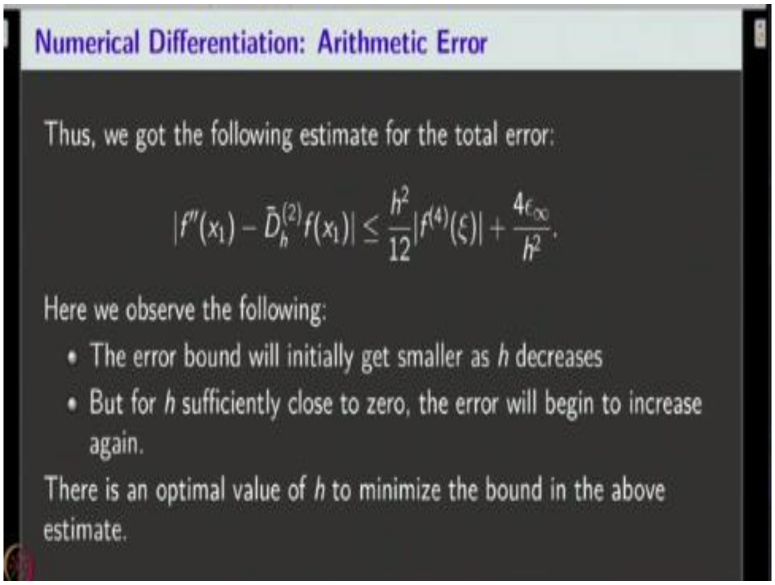
(Refer Slide Time: 24:57)



Now what you do is, you take the absolute value of the total error and that is given by this expression after taking the modulus. Now you use the triangle inequality to get this expression, that is the absolute value of the total error is less than or equal to $\frac{h^2}{12}\left|f^{(4)}(\xi)\right|$ plus you again take the modulus in the numerator. And apply the triangle inequality you will see that that is less than or equal to $|\epsilon_2| + 2|\epsilon_1| + |\epsilon_0|$.

And you just replace all these ϵs by the maximum value, then you will see that that is less than or equal to $4\epsilon_\infty$. Then you of course have a h^2 term in the denominator. So, that is what I am getting here. Therefore, when you take the modulus on both sides of the expression for the total error, you can see that the modulus of total error is less than or equal to this quantity.

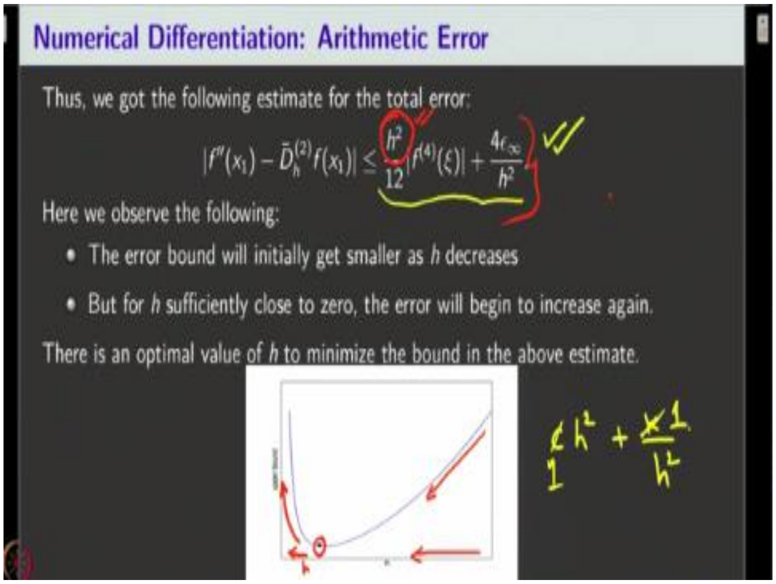
(Refer Slide Time: 26:15)



So, we have derived an upper bound for the total error. Now let us try to understand how this upper bound looks like. You can see that the upper bound involves a h^2 here, which will make the right hand side to decrease as h decreases. But it may not happen for h tending to 0, because after certain value of h, if you further decrease you can see that this term will start making the right hand side to increase drastically.

So, that is what I am writing here. The error bound will initially get smaller and smaller as you decrease h, because of this term. But as you keep on decreasing the value of h, then after certain value of h the second term will start dominating and it will take the right hand side to increase drastically. Therefore, there is an optimal h, beyond which the right hand side will start increasing rapidly as h tends to 0.

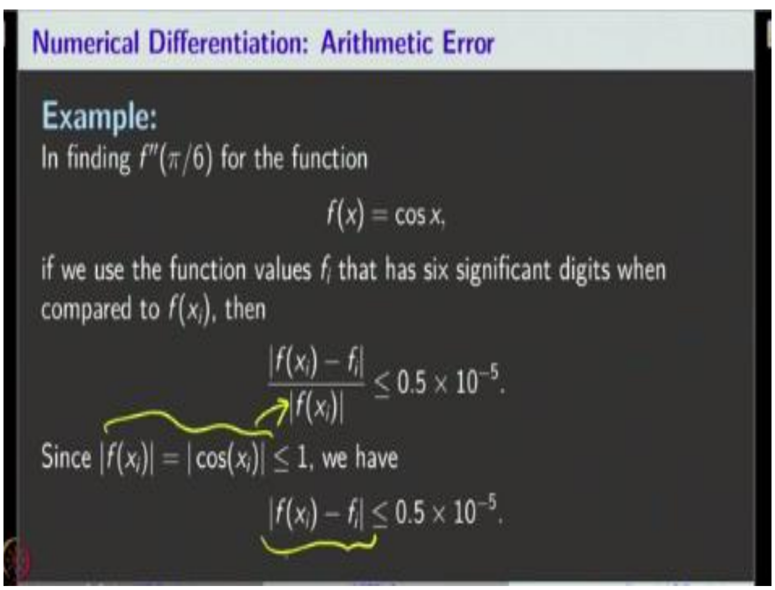
(Refer Slide Time: 27:35)



In fact, qualitatively you can see that the upper bound of the total error will look graphically like this. This is what I am trying to say that because of the first term you can see that as h decreases, the upper bound will start decreasing but this may not last for all $h > 0$. You can find an optimal h, beyond which if you start decreasing h, your upper bound will start increasing rapidly. So, this is what this expression tells you.

What I am doing here, is that I am just plotting the graph of constant times h^2 plus some other constant divided by h^2. You may even take c to be 1 and k to be 1 and its graph will something look like this. That is qualitatively how this function as a function of h will behave.

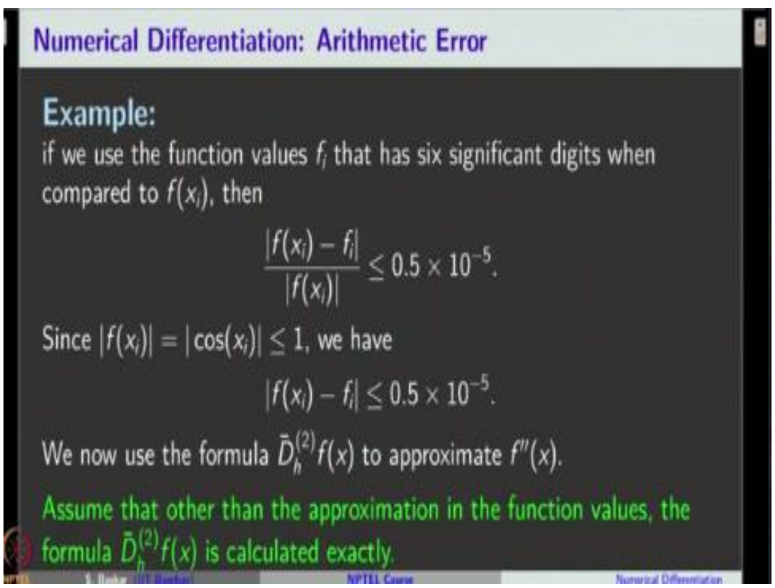
(Refer Slide Time: 28:40)



Let us take an example. Our interest is to find $\frac{f''(\pi)}{6}$ for the function $f(x) = cos\,x$. If you use the function value which involves certain approximation, then how the central difference formula will approximate the second derivative of the cos function. That is the question? To be precise, we will consider that the approximation f_i is obtained from $f(x_i)$ using six significant digits.

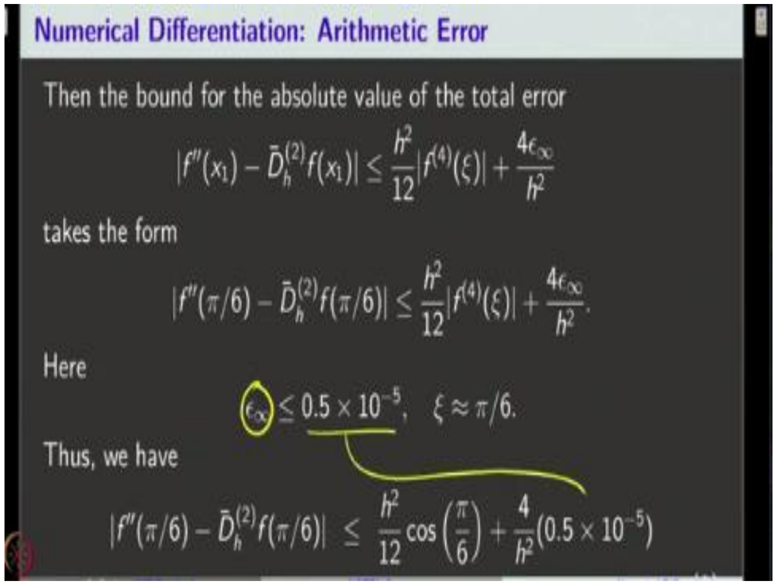
It means what, if you recall from our errors chapter, 6 significant digits means the relative error involved in f_i when compared to $f(x_i)$. It will be bounded by $\frac{1}{2} \times 10^{-5}$. Because you have six significant digits, if you have *n* significant digits, then it is - *n* + 1, that is why you have 5 here. Also, you can use the fact that cos function is always bounded between - 1 and 1 and from there you can see that the absolute error is less than or equal to 0.5×10^{-5}. I am just using this here and getting this estimate for the absolute error.

(Refer Slide Time: 30:15)



We will now use this information into the central difference formula evaluated with rounding error. Rounding error is involved only in the function value, that is, just for the sake of simplicity, we are assuming that the rounding error is involved only in the function value but not in the *h* value.

(Refer Slide Time: 30:38)

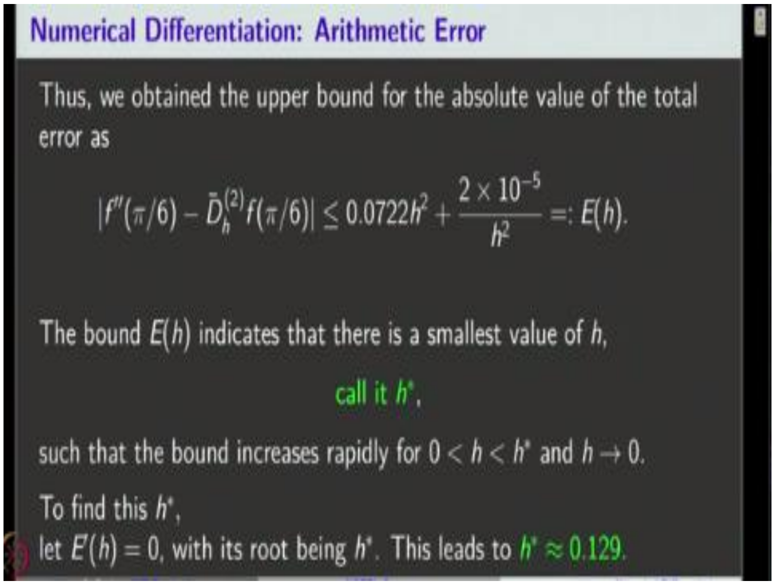


Then what happens is, if you recall the total error has the upper bound as this. In that now we will try to eliminate this because this is involving an unknown and also, we will try to get an estimate for this ϵ_∞, because we have assumed that the approximation in the numbers is just by six significant digits. So, with that you can see that ϵ_∞ can be taken as 0.5×10^{-5}.

And just to eliminate this what I am doing is, I am taking ϵ to be approximately $\frac{\pi}{6}$, why I took $\frac{\pi}{6}$, because that is the point at which I want to find the derivative of the function. You may use some other idea but I am just using this idea to eliminate this ξ. With that I can see that the total error is bounded by $\frac{h^2}{12} cos\left(\frac{\pi}{6}\right)$. This is a very crude approximation, actually plus 4 times ϵ_∞ is less than equal to this.

So, I will put this in the place of ϵ_∞ and that gives me precisely how this upper bound function will look like. This is an estimate now for me. Let me denote this estimate by $\mathrm{E}(h)$, it is a function of h.

(Refer Slide Time: 32:16)



So, we have the upper bound for the total error and we are using the notation $E(h)$ for that. Now, our interest is to find the optimal h. What optimal h means, optimal h means we want to find the value of this h, such that when you decrease your parameter h greater than that point, let us call this as h^*, when $h > h^*$, as you decrease h, n this region your total error will tend to decrease at least, its upper bound will tend to decrease.

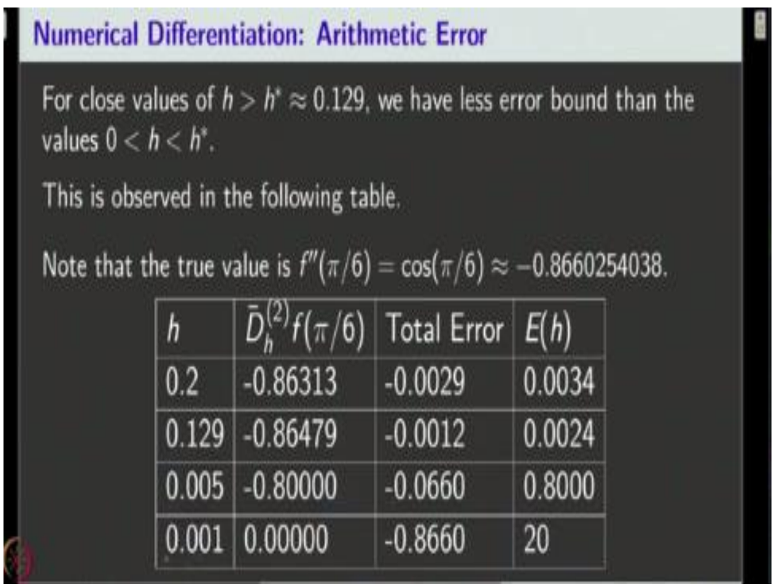
If you take h less than the optimal h, h^* then as you go on decreasing h your total errors upper bound will increase. So, we want to find this optimal h, how will you find the optimal h. Well, the graph of the function $E(h)$ will be qualitatively looking like how I have shown in the graph of the previous slide. Therefore, it is very clear that the optimal h can be obtained as the minimum of the function $E(h)$.

So, let us denote this optimal h by h^* and it can be obtained by finding the minimum of this function. So, that optimal h is such that the upper bound will increase drastically if you go on reducing h in the region 0 to h^*. That is the danger of, you know, go on decreasing the parameter h believing or thinking that you will get better and better approximation. No, it is not true if we are putting these formulas on a computer then there is a limit beyond which you cannot go on decreasing your h.

That is the moral of this story. Let us see what is this h^* in this particular example. To find that, you have to find the derivative of this function $E(h)$ and see where that derivative vanishes. This is a simple and well-known technique introduced in the calculus course, how to find maximum and minimum of a function. Using the technique, you can find this h^* and in this example that h^* is given by 0.129.

So, remember if you take h less than 0.129 and from there if you keep on decreasing the parameter h then the upper bound of the total error will increase, that is what we are seeing. That does not mean that the total error should increase. But unfortunately, it will also increase in this particular example.

(Refer Slide Time: 35:14)



What I am doing is, I am taking $f''\left(\frac{\pi}{6}\right)$. Remember, $f(x)$ is taken to be cos x, therefore $f''\left(\frac{\pi}{6}\right)$ is given by this number, up to some 10 digits I am taking. And now let us see how this central difference formula will approximate the second derivative of the function f, that is cos function. When you compute these values on a computer, I am just taking $h = 0.2$ which is greater than the optimal error in this example, well the value obtained for $f''\left(\frac{\pi}{6}\right)$ using the central difference formula on the computer.

That is why I am putting a bar there, because it will certainly involve the arithmetic error. And computer gave us this value which is pretty close to the exact value. I mean this is also strictly speaking not the exact value but this is the value with better accuracy than this value. That is what it means and when compared to this value this approximate value has the total error like this and the upper bound has the value this.

Remember the upper bound expression is given like this. So, you can plug in h in this expression and get the upper bound value also at $h = 0.2$ and that is given like this. Now let me take $h = h^*$, that is the optimal value of h. With that h, your central difference formula gives this approximation. The total error involved in it, is this. Well, you can see that from $h = 0.2$ to $h = 0.129$. The total error decreased as we expected also the value of the upper bound also decreased.

Let us go ahead and choose a h less than the optimal error and see what happens. Now I am choosing h as 0.005 which is less than h^*. You can see that the value of the central difference formula for the function $f''\left(\frac{\pi}{6}\right)$ is given like this. The total error you can see that it increased from what you have got for $h = 0.129$. By reducing the value of h, we got a bad approximation.

But theoretically when you take h tending to 0, you are supposed to get better and better approximation but numerically when you compute on a computer, the situation is different. That shows that computer is now started making significant error in this calculation coming through the rounding error. You can also see that the upper bound has drastically increased. I have further gone ahead and took $h = 0.001$.

Well, I am decreasing h therefore mathematically, I should get better approximation for the second derivative using the central difference formula. But my central difference formula gave this as the value and therefore what is the total error involved in it is really almost 100 percent error it gave and the upper bound value is 20. So, that is the danger in dealing with the computation especially when you do on a computer you have to be very careful.

Mathematically it may be that when you go on decreasing certain parameters you will get better and better approximation. But it may not be the situation when you go to implement these methods on a computer. One has to carefully understand the error analysis both from the mathematical point of view as well as from the computation point of view. With this note, let us conclude this lecture, thank you for your attention.