Numerical Methods and Simulation Techniques for Scientists And Engineers

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Lecture 08
Numerical differentiation

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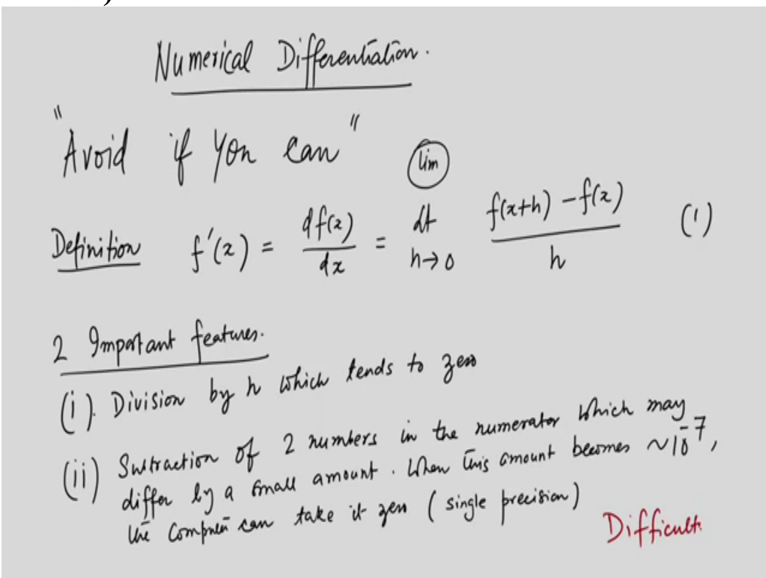

So, what we are going to discuss today and maybe the next is well is numerical differentiation. So, all of you are familiar with the concept of derivative. You have taken it in a number of you know situations in which you are to either minimize a function or find the slope of a line or you know find that where the function has a extremum point. And have also taken second derivatives and so on which shows the curvature of a function and maybe the third derivative that is f triple prime so to say which shows the you know the skewness of the function and so on okay.

So, you have seen all that in a variety of contexts throughout your academic career and here we are going to talk about taking derivative in a computer may be from a set of data points and you may actually want to take a derivative at a given points or in the neighbourhood of point. And how to go about doing that is what we are going to discuss. The first thing that can be said about numerical differentiation is that is that avoid if you can that is if it is avoidable to take a derivative in some form.

That is sometimes we will see that integral equation or a differential equation can actually be converted into an integral equation. And integration is a much better thing to perform numerically than a differentiation. So, we wish to caution every participant and every student that numerical differentiation is a risky thing because of a number of points and we highlight the most important of them.

That is the so in order to understand that let us go with the definition, so the definition of derivative. So, the definition goes as f prime x which is all known to you and it is equal to a df dx so say f is a function of a single variable x and it is a limit which you can also say as lim if you like this is also used in some books lim or I will use lt and there is for the limit. And it is f x + h - f of x divided by, so h is a small number which displaces the function f of x by a small amount such that f of x + h is defined in the neighbourhood of f of x.

And so it is a difference between the 2 functions at x + h and at x divided by h all of you are very familiar with this now the problem lies right here. So, let us just talk about give it a name as equation one and 2 important features of this is one being the division by h whose limit goes to 0 or rather which tends to 0 as said in the definition itself. So, you are trying to divide it by a quantity which is negligible or which is in the limit it goes to 0.

And also not to forget that the numerator is also somewhat tricky because you are taking the values of the function at 2 very nearing points and if this value that is f of x f of x + h - f of x it becomes a very small number to the tune of 10 to the power -7 or -8 the computer will automatically take it to be 0. So, there will be a 0 by 0 division which is not something that the computer can handle. So, this subtraction of 2 numbers in the numerator which may differ by a small amount.

And when it becomes this amount becomes of the order of 10 to the power -7 or -8 the computer can take it to 0 something that happens in this single precision. So, when you are working with single precision this is what happens any number that falls below 10 to the power -7 or it becomes of the order of 10 to the power -7 the computer takes it as 0. So, basically it is a problem from both sides that you are dividing it by a small number and sometimes the numerator becomes so small that the computer takes it as 0.

Or it because both can be operative simultaneously which means that you will have a 0 by 0 situation or something that limiting in the limiting case tending to 0 divided by another quantity that in the limiting case tending to 0. So, this is why the derivative or taking a derivative in a computer is a risky you know thing. So, it is a basically what we wanted to say is that there is a difficulty.

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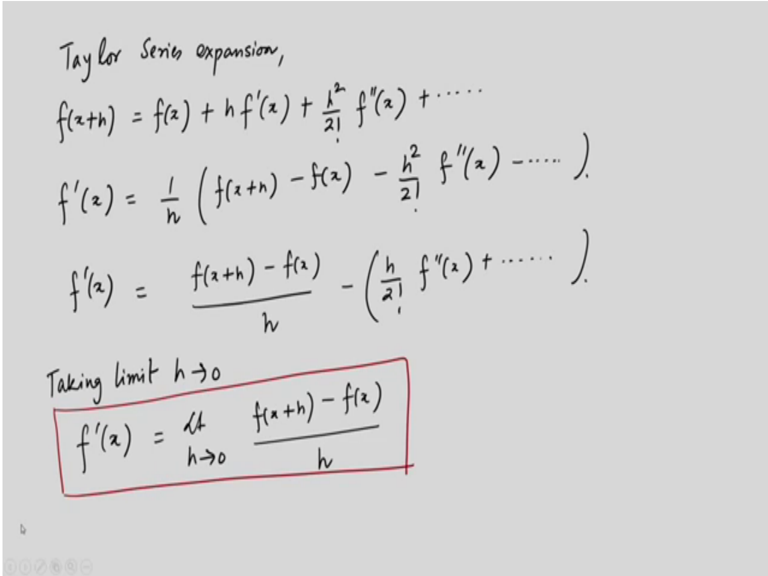

So, let us see the method of taking derivatives I mean when I say it it is risky does not mean that we never take derivatives we often have to take derivatives for calculating slopes or trying to minimize a function. So, the method of derivatives taking derivatives is best illustrated by a Taylor series expansion. So, where we expand a function in the neighbourhood of f of x by the first derivative multiplied by this h and evaluated at of course at that point if at x equal to some point.

We are taking it as x but it is some particular point of x which could be x 0 and then h square by 2 factorial f double prime x and so on. We have h cube by 3 factorial f triple prime x and so on so which we will see. So, if we try to compute f of f prime of x which is equal to 1 over h f of x + h - f of x and - h square by 2 factorial f of double prime x and so on. So, this the first term can be taken out which is f of x + h - f of x divided by h and a - h over 2 factorial f double prime x and so on ok.

So, we will have so as you understand that the first term came in the definition of f prime of x that you have been familiar with but so you are missing out a factor which is which is the double derivative and times this h and so on. So, both the problem that is missing out the justification of the rationale behind missing out the second term which comes inside the bracket the first bracket can be justified if we take the limit.

So, basically what I am trying to say is that taking limit h tending to 0 you have the original definition that is f of x prime equal to limit h tending to 0 f of x + h - f of x divided by h and you are also allowed to leave out the second term because your h tending to 0. So, this term is simply multiplied by h so that can be neglected so we get you get back the usual original definition of the derivative, so ok.

So at this level f prime of x at this level itself it looks like similar to the original definition and it exactly becomes the original definition if you take the limit. So, this is what I am trying to say all right. So, this is the thing that we do and so that is the definition and so on. So, let us box this thing so there are better methods more accurate methods of calculating derivatives ok.

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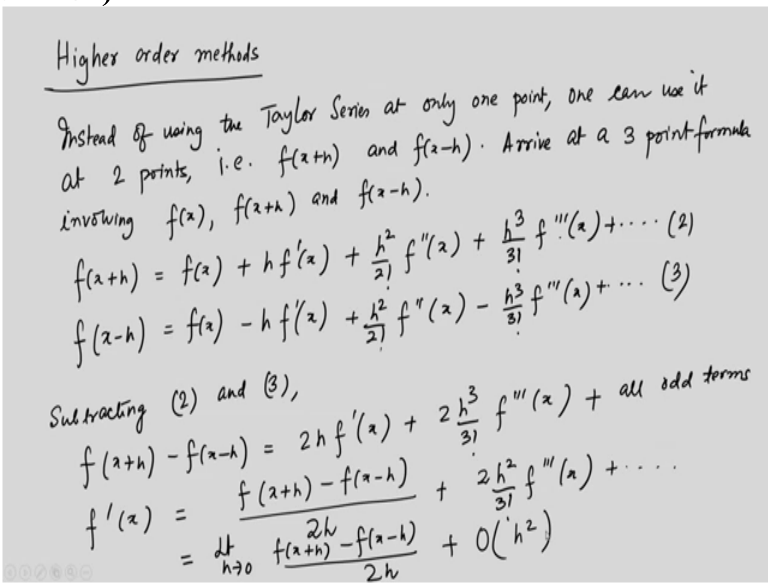

So, let us call them as higher order methods of calculating derivatives okay. So, the higher order method is that we can use instead of a forward difference we can I use what is called as the you know the divided difference method. So, what I mean by this is that so instead of using the Taylor series at only one point, one can use it at 2 points that is f of x + h and f of x - h so I am using 2points on both sides of f of x differing by the same amount h.

So, take 2 points f of x + h and f of x and we will arrive at a 3 point formula which is involving f of x f of x + h and f of x - h so f of x + h is equal to f of x + h f prime of x + h square by 2 factorial f double prime of x and so on ok. So, that is your f of x + h which is what we have seen and f of x - h is simply f of x and a - h of f prime of x and we have a + h square by 2 factorial f double prime of x and what we do is that we will add both of them rather subtract both of them because if you add then and this f prime goes away.

Now we do not want that to happen so subtracting let us call this as 2 and this is 3 f of x + h - f of x – h. So, this the f of x will get cancelled out and this will get added up, so it will be 2h f prime of x + 2 factorial becomes simply 2 and if I subtract them then of course this term also gets cancelled out and we have another term which we are not written let us write that term explicitly because this is the next correction that comes.

So, it is h cubed by 3 factorial and f triple prime x and this comes with a - h cube by 3 factorial f triple prime x and this is plus and so on and this is also plus so on ok. So, this becomes equal to twice of h cube by 3 factorial 3 factorial is nothing but 6 and then there is a f cube it is a triple prime which means it is a third derivative of f with respect to h and all odd terms which we have not written.

Now this is going to only detain the odd terms because the even terms are going to cancel out when you take the subtract one from the other. So, if you write down the difference or rather if you simplify this, this becomes equal to f of x + h - f of x - h divided by a to h and 2h square by 3 factorial f triple prime x that is the leading order and of course all other terms. Now you see that if I take the limit then we are going to have only seeing out terms which are h square and not h as we have done it in the earlier case.

Okay so this is meant by a higher order or more accurate quantity of or rather quite a more accurate definition of this so I will write it as limit h tends to 0 f of x + h - f of x - h divided by 2 h + are terms that are of the order of h square. So, if you look at this earlier definition we have missed terms which are of the order of h here okay in this step and now we are missing out things of the order of h square and since in the limit h tending to 0 h may not be neglected but h square can certainly be neglected with you know better confidence okay.

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$$\boxed{f'(x) = \mathop{Lt}_{h \to 0} \frac{f(x+h) - f(x-h)}{2h}}$$

Likewise a 5-point formula yields,

$$f'(x) = \frac{1}{12h}\left[f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)\right] + O(h^4)$$

$$\boxed{f'(x) = \mathop{Lt}_{h \to 0} \frac{\left[f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)\right]}{12h}}$$

It is more intuitive to represent it as,

$$f_1 = f(x-2h) + 8f(x+h) \; ; \; f_2 = 8f(x-h) + f(x+2h)$$

$$f'(x) = \mathop{Lt}_{h \to 0} \frac{1}{12h}(f_1 - f_2).$$

So this thing let me write it neatly so f prime of x is equal to limit h tending to 0 f of x + h and f of x - h divided by 2 h and we are only missing terms of the order of you know h square so this is the definition it is a better definition uses 3 points and it is also known as the divided difference okay. Likewise 5 point formula I show this without proof but you should be able to do it so you write f of x + 2h and then expand it you write x f of x + h expand it and then of course you do some algebra.

In order to do it to convert it rather to a definition of f prime of h and that comes out as so f prime of x this is equal to 1 over 12 h and f of x - 2h – 8 f of x - h + 8 f of x + h - f of x + 2 h and you know what you miss out is something of the order of h to the power 4. So, you are only missing out terms which are h to the power 4 and if h is small it makes absolute sense to miss out that top. And you see that you have involved 5 points namely the f f of x + 2h f of x + h f of x - h f of x - 2h and of course f of x which appears there and this has to be divided by 1 over 12 h.

So, the definition of this derivative is limit h tends to 0 and f of x - 2h - 8 f x - h + 8 f x + h - f of x + 2 h and divided by 12 h and this is the definition of this ok. So, this is the f prime of x that makes it once again okay. So, these are definitions all right we are only seeing it formally for now and we will see that how things can be you know sort of applied to various physical situations.

So, if you it is more intuitive to represent it as f 1 define quantities which are f 1 which is x - 2h + 8 of f x + h and define another one which is f 2 which is 8of f x - h and + f of x + 2h and then you can write this derivative as limit h tends to 0 1 over 12 h and f 1 – f 2 ok. So, what it has you know the advantage that it has over this slightly larger form of this is that it is it reduces the number of operations even plus minus are operations that have to be performed by the computer.

And this only finally if you do this or rather fragment these operations of taking additions and subtractions into this f 1 and f 2. So, you calculate this f 1 which is just a sum of 2 numbers and this is again the sum of 2 numbers is f 2. And then finally you take one difference one subtraction f 1 and f 2 and that will give you the f prime of x ok. So, this is more slick definition and is also very useful.

So, let us quickly touch upon the errors that have been introduced so far into or while taking this numerical differentiation we have cautioned the readers and the participants of this course that numerical differentiation or a derivative is somewhat risky to take.

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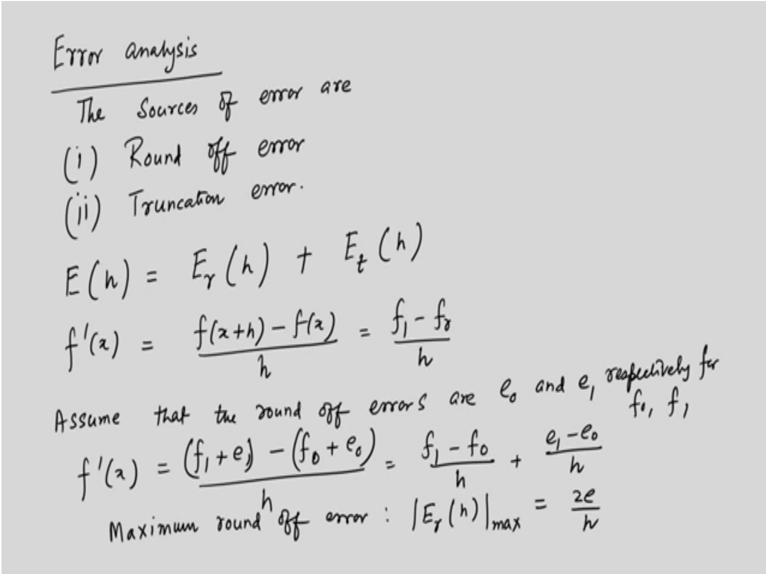

And so let us do an error analysis, so one source is the sources of error are one, round of error okay and 2 truncation errors okay. so, in the numeric when we do it there is always a truncation that we do after so many decimal points okay. And we take only the significant digits thinking that that is going to give us the right result and we do not always worry about 8 decimal places or 16 decimal places as the you know the precision would actually give us.

So, there is a round off error and when you are doing it iteratively that is you are passing on one you know the data or the values obtained in one iteration to the next iteration and then to the next iteration and so on. These round off errors can become quite important. Second which is also very important in this particular case is the truncation error. We are leaving out terms with the order of which our order of h or which our order of h square or which our order of h cube in this particular case no h cube but h for h h square h for and so on.

At least to the extent that we have shown they all contribute to the errors that produce. So, we write this error E as a function of h, h being the derivative the smallness parameter in this particular case is E r h where our resort or rather represents round off error and + Et h where t denotes the truncation error. So, let us see the same forward difference formula take this one it is equal to x + h - f of x divided by h it is equal to f 1 - f 0 divided by h and so on.

So, this is the definition of the function so we call it f 1 and f 0, so that is the function we define them as so assume that the round of error e 0 and e 1 respectively for f 0 and f 1 so what it means is the following that your f prime x is actually f 1 + e 1 we are neglecting that - f 0 + e 0 again we are neglecting that divided by h. So, we have taken it as f 1 - f 0 by h and a + e 1 - e 0 by h looks like that they are getting subtracted but they are not if you take the maximum one so the maximum round of error is the following.

E r h and this is the maximum these 2 errors will add up and will give me some e which is of the order of e 1 and e 0 and you give me twice of e over h cross okay. So, that is the round of error or the maximum round of error okay. So, we have dealt with one type of error which is round off let us see the truncation as well.

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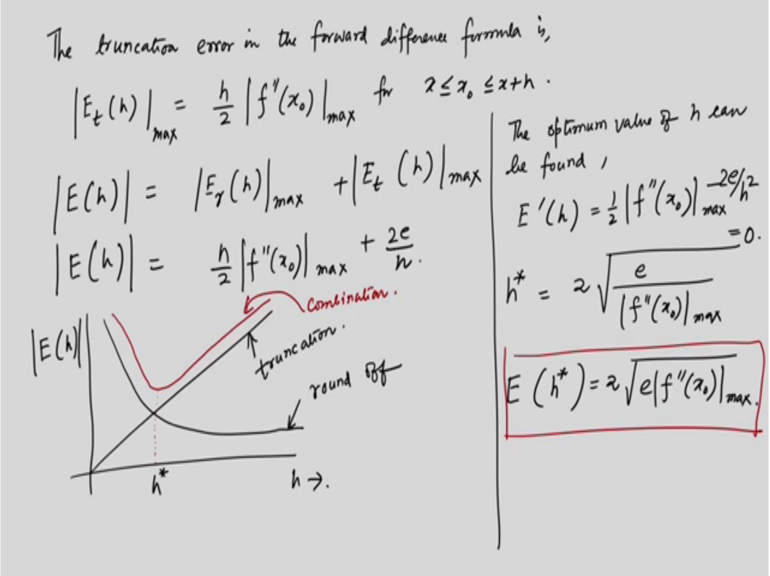

In this particular case as you know the truncation error is only of the order of h. So, this is nothing but h over 2 and f double Prime and we call it let us call it an x0 magnitude of that is a double derivative where x 0 is some point between x and x – h, so x < x 0 < x + h ok. So, we are taking it at a say a midpoint between x and x + h we are trying to calculate the derivative there. So, the total h or the magnitude of h is the sum of both so it is like E r h rather with the max so this will go with a max it is a maximum error if you say.

So, this is the maximum derivative or rather double derivative evaluate maximum value of the double derivative evaluated at this point. So, this is this + E t h and max of that now this is nothing but h over 2 f double prime x 0 evaluated. So, there is a maximum of that and there is a 2 e over h ok. So, it is a very interesting the error has an interesting dependency on h for the first term it increases linearly with h whereas for the second term is goes as a hyperbola that is it goes over as a 1 over h. So, if you try to plot that then one of them will be like this so this is like the truncation one. And the other one is one over h so this is like this round off, so this is your e as a function of I mean this is e h as a function of h.

So if you add both of them it will look like something like that so let me draw it with a different colours so that that is the resultant. So, it goes like this and then it goes like this okay. So, there is what it says is that there is a minimum or rather of this plot of this red plot which is the combination so this is the combination of that. And this combination goes through a it has a non monotonic dependence and it goes through a minimum.

So if you can choose your h value at this minimum point then your error will be minimized okay and so this is the whole idea of this so h should not be large it should not be too small it should be some optimal value. And how do we find out that optimal value this is so let us do it here can be found using your e prime h taking a derivative and putting that equal to 0. So, this is that f double Prime at x 0 the maximum of that and - 2e over h square.

And put that equal to 0 okay so this h opt or let us call it h star call this point as h star, so h star is nothing but 2e over f double prime x 0 and the maximum value of that and so this is actually nothing but, so at this value of h if you put this on the earlier step then e at h star why am I writing this, so this is taking a a prime so this e at h star just would not have this, so I have taken a derivative here now I am writing it e as a function of; so I will put that here in this expression and put h equal to h star there so this is equal to a 2 e f double derivative and so on f and this is that max.

So, if you know these values that is if you know the error that is a round of error that is if you are taking say 4 significant digits or 5 significant digits then you know that what is the round of error for this caused by this you know curtailing it at this up to 4 or 5 decimal places. And the f double prime is the curvature of the function at that value between x and x + h then you can get an idea of this what would be the error.

This can only be computed for a given particular problem okay and this is what we have shown.

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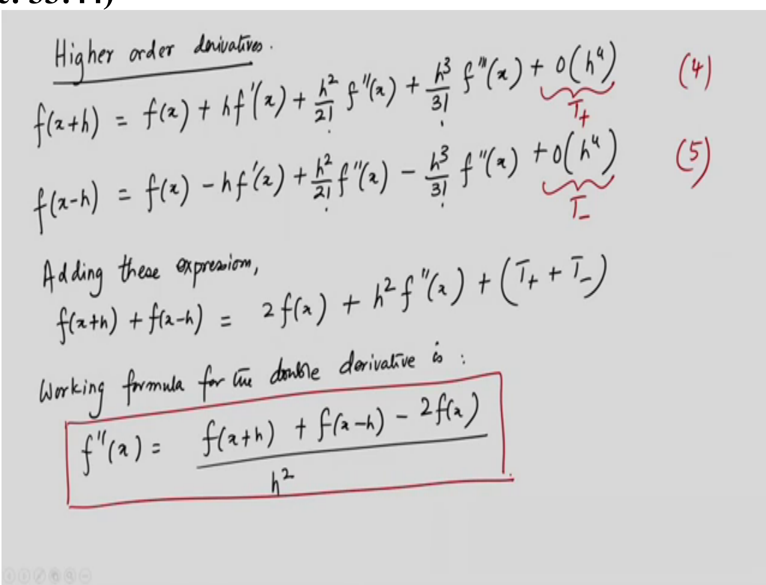

Let us quickly look at now the higher-order derivatives. So, we have talked about a better approximation more accurate approximation but for the first order derivative now let us look at the higher-order derivatives. So, I need at least 3 points I mean a higher order derivative cannot be done with only 2 points. So, we have to take a f of x + h which is what we have done earlier. So, take a Taylor expansion of f of x + h in the neighbourhood of f of x h is small and f prime so this is the first term the second term is this double prime.

And of course the next term is this and of the order of h 4 is what you are missing okay. And f of x - h similarly is f of x - h f prime of x + h square by 2 factorial f double prime of x - h cube by 3 factorial f triple prime of x and again I am missing out h 4 okay. So, let us call these things the truncation that we are doing let us call this as the p + because we have obtained it from fx + h and let us call this as t - which we have obtained from f of x – h.

Now I am not going to subtract them because if I subtract I will have the f prime surviving and f triple prime surviving. Whereas I want the f double prime to survive and all the odd terms in h or the odd derivatives that is f prime f triple prime and all that to go to 0. So, we will add these 2expressions and let us call them as what would we call them earlier so anyway we had only used up till 3.

So, we will use 4 and 5 for this so this adding these expressions f of x + h + f of x - h it becomes equal to 2 f of x which is of course there and h square f double prime x and then whatever we are missing out as T + + T - and so on okay. So, the working formula for the double derivative is f double prime x is equal to f of x + h + f of x - h - 2 f of x divided by h square ok. And so of course so this is the h square and you can put h limit h tending to 0 so the truncation error in this particular case Et h ok, let us do it in the next page let us box this expression which is the working formula.

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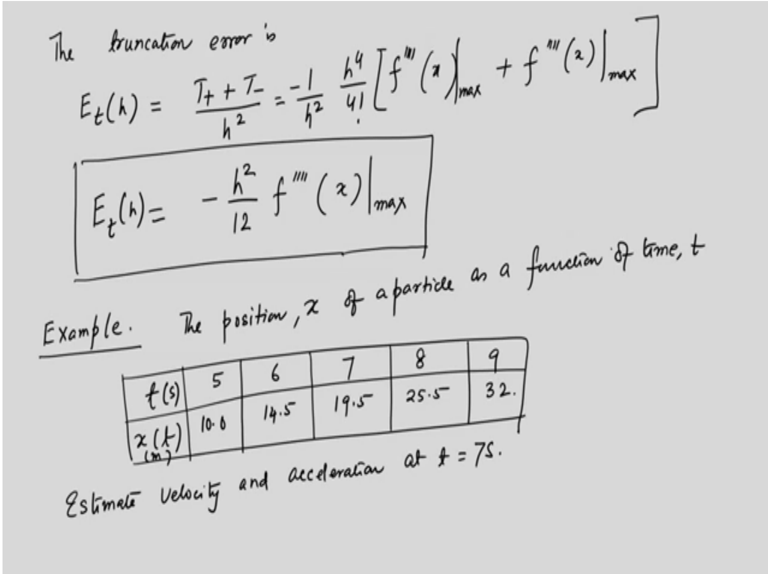

E t h the truncation 1 is T + + T - divided by h square which is nothing but equal to - 1 over h square h to the power 4 by 4 factorial and f 1 2 3 4 at x 0 and the maximum value of this or rather we can simply write it as f of x and its maximum value. And you know f of this and its maximum value whatever it is evaluated at point which is between x between x and x + h or x and x - h for this but 2 terms respectively.

So, this is that between x and x + h and this between x and x - h so if you add both of them they are so the truncation error is only of the order of h square and so we have just simply added these 2 terms and 4 into 3 is 12 4 into 3 into 2 it is 24, so there are 2 terms so 2 and 24 will cancel and give you a 12 in the denominator. So, this is the truncation error and so on ok so that is, so if you remember the or truncation error was of the order of h in the previous case where we have computed the first derivative okay.

So, you know sort of you have you can have many examples from here and let us see one simple example. So, let us say that a particle is you know as an example see the velocity or rather the position of a particle as a function of time x of a particle as a function of time t is shown here okay. So, this is a; so this is your you know so your t and x as a function of t so this is 1 2 3 4 and so on okay.

So, this is 5 6 7 8 9 and so on, so t in seconds and this is probably in meters okay so in meters. So, it is 10.0 and 14.5and nineteen.5 and the 25.5 and 32, so this is the distance that is you know given. So, you estimate the velocity say estimate velocity and acceleration at t equal to 7 seconds okay either way simple problem and so on. So, if you do it by 3 point and a 5 point etcetera formula so let us just take a 3 point formula which is also called as a divided difference method.

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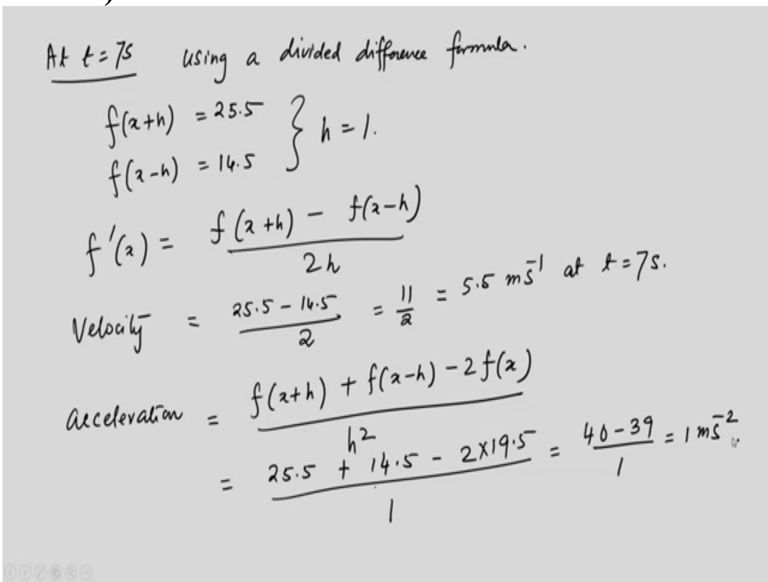

So, at t equal to 7 seconds using divided difference formula so you see that f of x + h is 25.5 and f of x - h is 14.5 and h is equal to 1 so f prime is equal to f of x + h - f of x - h divided by 2 h which is simply equal to 25.5- 14.5 divided by 2 which is 11 over 2 which is equal to you know 25.5 meters per second at t equal to 7 seconds and similarly you can calculate the double derivative in order to calculate.

So, this is the velocity okay and you can calculate the acceleration using this formula which is f of x + h f of x - h and f of x divided by h square, so the acceleration is f of x + x + h + f of x - h - 2 of fx divided by h square and so h is equal to 1 so f of x + h is of course given as 25.5 + 14.5 - twice of what is f of x 19.5, so 2 into 19.5 divided by 1 so this becomes equal to 25 + 14 becomes 39 and 40.

So, this becomes 40 - 39 by 1 which is equal to one meter per second square okay. So, it is you can write it as 1.0 a very simple problem we will see more complicated and more you know sort of applied problems in the next lecture of the discussion.