Numerical Methods and Programming P. B. Sunil Kumar Department of Physics Indian Institute of Technology, Madras Lecture - 25 Numerical Derivations

You remember the problem we were discussing in the last class was the computation of derivatives numerical the numerical computation of derivatives given a set of data of points and you have given a set of data of points which is coming from some other calculation or from an experiment. So given by some other functions you had a set of data of points and you want to compute derivatives in between or on any of this data points.

You may want to evaluate the derivative of this somewhere in between or even on one of the data tabulated data points. So we have discussing cases where that is only one dimensional function of one variable and so one way we said that which we can compute this derivative by constructing an polynomial which interpolates this points okay and then take the derivative of that polynomial and then we will looked at what will be the error in the polynomial the error in the derivative because is easy to compute this way because we know that the error in the interpolating polynomial is like the next term in the polynomial. So the derivative error in the derivative would be the error in the next term that is what we looked at last in the last class.

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Okay this summarize we said that, we could given a set of data of points we know how to construct a polynomial of order n which passes through n plus 1 points and starting from x_0 to x_n . So n plus 1 points we know how to construct this polynomial and the advantage of writing in it this kind of Newton forms that is what called newton's form polynomial is

that we this coefficients of this term that is f of $x_0 x_1$, f $x_0 x_1 x_2$ is the coefficients of the polynomial of the terms of order 1, 2 etcetera can be constructed rather easily a from a difference tables is algorithmically efficient way of doing it so this is useful form for the polynomial of the polynomial to construct the derivatives that is what we look at in the last class

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So then we said that the derivatives of this polynomial now then once we have the polynomial of that form and the derivatives can be written in this fashion, so look at the second order term. So we had a first order term now the derivative this does not appear in the derivative being a constant and here this is the first term in the derivative would be just f of $x_0 x_1$ right and the next term would be f of $x_0 x_1 x_2$ with the first order term that will be the x minus x_0 plus x minus x_1 that is the term and then we have the error term, the last term we have an error term which we can evaluate because we know this term is derivative of the next term in the polynomial that is n plus1term in the polynomial that is what the error term is okay that is can be evaluated.

so we get that as this one some function we get that as something the order of n plus 1 some derivative of the order of n plus 1 of some function and multiplied by x_i minus x_j , a product of x_i minus x_j for all j value which are not equal to i so now this form is valid is strictly valid only when the error is evaluated at one of the tabulated points and if the error if you want to evaluate the error at non tabulated point then we have one more term which is actually the, this multiplied term the derivative of this function which is we said it is difficult to evaluate or impossible to evaluate in the sense because we do not know the functional form of this.

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So basically this form of the error give us a qualitative idea what the error is and most of the cases we will not able to say what this term actually the order of the where the magnitude of this term which is we can say that nth order of n plus 1 derivative is but we saw that if you have a set of data points in between we saw that set of data points.

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Let us we say, we have many data points and you want to compute in derivative here at any point in between let us we say, we want to compute derivative this value of x and then and then it is not necessary to take the whole polynomial which goes through the whole set of data points. So we could actually construct a polynomial here which goes through these 3 points and then take the derivative.

So this way, we can actually get an exact, we can actually get an exact measure of the error because we can actually take this polynomial this point also and construct another polynomial okay which goes through all of this 4 points and then take at look at the derivative coming from that.

So the difference between the polynomial which goes through these 3 points lets called that as p_3 of x and the polynomial which goes through so, this will be p_2 of x_3 points 2 and the polynomial which goes through 4 points it gives as p_4 of x_i will take the derivative of these two and the difference between these two derivatives is evaluated at this point will give as the error in the p is once again p_3 at this the error in the derivative p_2 because the error in the polynomial p_2 is like the next term it can get from p_3 . So that is what we looked at and found this is this is gives as very good approximation, very good idea about what the errors in the derivatives are.

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So that was the case with the newton's form of the polynomial okay that is polynomial of using this polynomial of this form okay and then take the derivative of this and you remember what is f of x_0 , x_1 was okay, so we could construct i set of data points will call them i 1, 2, 3, 4, 5 etcetera and then we had the x_i values which is x_0 , x_1 , x_2 , x_3 , x_4 , x_5 and then we had a f of x_i values okay that was given here f of x_0 , f of x_1 , f of x_2 .

Okay now, this was given to us in the form of set of tabulated set of data and we could construct this coefficients as f of x_i right as f of x_i basically this point itself that is same as f of x_0 , f of x_1 , f of x_2 , f of x_3 , f of x_4 , f of x_5 . So that is f of x_i and then we had f of x_i , x_i plus 1 that is the next term in the thing which we said is given by f of x_1 minus f of x_0 divided by x_1 minus x_0 and f of x_2 minus f of x_1 divided by x_2 minus x_1 and f of x_3

minus f of x_2 divided by x_3 minus x_2 and we had f of x_4 minus f of x_3 divided by x_4 minus x_3 and the last term would be f of x_5 minus f of x_4 divided by x_5 minus x_4 . So we could construct that.

Okay, so that is is the difference table which we construct and then we could take the next one would be then difference between these 2 divided by this term now simplify I will write remembers this as f of x_0 , x_1 this is x_1 , x_2 the next term would be f of $x_2 x_1$ minus f of this is square bracket remember, distinguish between the square bracket in this bracket x_1 , x_0 divided by now x_2 minus x_0 and here next would be f of this will be $x_3 x_2$ minus $x_2 x_1$ by x_3 minus x_1 and here you will have the next term f $x_4 x_3$ minus f $x_3 x_2$ divided by x_4 minus x_2 last here would be $x_5 x_4$ minus f $x_4 x_3$ divided by $x_5 x_3$.

Now we can construct further okay taking the difference between these two then it will be the denominator would be x_3 in this case of x_3 minus x_0 and it goes further like that because next term will have a denominator x_3 minus x_0 here and it will have x_4 minus x_1 , x_4 x_5 minus x_2 you can construct a difference table of this form. So that is what we had so these two went to that, so we had a difference table constructed in this fashion okay now this will go to that and these will going to that.

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So this difference table what gives the advantage in this particular case that we must have a difference table and whether it is a polynomial or its derivative, we can write that in terms of this coefficient by reading of by reading of these coefficients, okay now if I am starting, if I am entering difference table at this point that is entering the difference table at that top okay and then i have the coefficients the first term would be just f of x_1 is f of x_0 and the next coefficient of the next term would be f of $x_1 x_0$ and then f of $x_2 x_1$ minus f of $x_1 x_0$ by x_2 minus x_0 . So that is what we have written as this term here, so this is actually entering the entering the difference table in the top okay but I said that if you want to evaluate it derivative at any point in between there is no need to enter the difference table from the top we could enter the difference table somewhere in between okay, what I mean by that is if I want to evaluate the derivative of derivative if I want to get the derivative of the function had some value x where x is lets say larger than some x i okay x_i is the larger than the x_i and then I could actually enter the difference table at that point x_i . So let me say that this point here and construct a polynomial this way or around that may be entering here constructing a polynomial. So I could enter the difference table principle any where which contains the point x such that it contains the point x, so in this case I could construct, so here I had 5points 1, 2, 3, 4, 5 let us say 5 points and I want to construct a derivative of the point here evaluate the derivative here.

So I could use a linear polynomial by just taking two points I could just take the constructed a linear polynomial derivative of that will be the constant, okay that is the linear polynomial by construct by entering in to that difference table at this point the third point okay that is 0, 1, 2 here. I would enter here and then the first my polynomial would start from f of x_2 . So then my polynomial would be f of x_2 plus f of x_3 minus f of $x_2 x_3$ minus x_2 into x_3 minus x_2 .

So that is what we saw yesterday, so that is the way of constructing the polynomial and the derivative okay so if I want it here that is $x_0 x_1 x_2$ so in between x_2 and x_3 I want to find the derivative okay and decide to take the linear polynomial between which connects these two points as a straight line that I would construct it as, so p of x as now f of x_2 that is my first term in the polynomial that is f of x_2 it will be entering here okay and then I would entering here first term f of x_2 and the next term would be f of x_3 plus f of x_3 minus f of x_2 divided by x_3 minus x_2 in to x minus x_2 that will be my, that is my polynomial okay.

So it is a f of p of x is f of x_2 plus f of x_3 minus f of x_2 by x_3 minus x_2 because this is my coefficient $x_2 x_3$ which comes in here okay that is my polynomial okay and then I can take my derivative of that would be simply f of x_3 minus f of x_2 by x_3 minus x_2 actually connecting a straight line through a slope of a line that is way I can construct this

Okay so now, we need an notation for that we normally write it as what we called as p_i of x, p_i of x will have to denote here or we write the difference table will put an i this is to say where it which point in the in the difference table are we entering, okay so now I can construct the same derivative here okay evaluated the same derivative here by constructing a second order polynomial, okay now this is the first order polynomial I could construct a second order polynomial but there are 2 ways of doing it by entering the difference table here okay and write it to the next polynomial here.

Okay now this is linear next term would be taking this coefficient, okay first term is this I entered here okay I enter at this point this point okay I have the first term is this second term is second term this is coefficient linear term and this will be the coefficient of the quadratic term. So that will be the f of x_4 minus f x_4 x_3 minus f x_2 x_3 divide by x_4 minus x_2 in to x minus x_2 in to x minus 3

So that will be the next term that is one way of doing it or I could say that I would enter okay here I enter this point okay then construct a polynomial goes to that, that also give me a second order polynomial. So then I would enter here and my term would be f of x_1 plus f of x_2 minus f of x_1 by x_2 minus x_1 into x minus x_1 now because I entered a x_1 okay then the next term which will be x minus x_1 into x minus x_2 there are two ways there are many ways now right now if you constructing only linear polynomial that is only point where we can enter to construct a polynomial but if your doing a second order polynomial is quadratic polynomial that will be the 2 ways we can enter here or here.

Okay now we see the possibility goes up if constructing a higher order polynomial to be evaluate the derivative but the major point I want to say is that you have to remember which point in the difference table you have entered and it should keep in mind that construct this when you make the algorithm. So we will see the implementations of this algorithm in later class.



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Okay that is now the newton's form with x_0 , x_1 , x_2 , x_3 tabulated um in a difference stable, so now the difference between the difference x_0 minus x_1 , x_1 minus x_0 , x_2 minus x_1 , x_3 minus x_1 etcetera that could be very different there is no need of there is no need of in this particular form there is no need to restrain that differences that could be any value but we have seen earlier in our interpolation when your looking at the interpolation case that its advantages of the algorithm much gets simpler when you look at, when you look at tabulated points at equal distance that is x_1 minus x_0 equal to x_2 minus x_1 equal to x_3 minus x_2 equal to some value h. So in that case even though, obviously the whole algorithm is much simpler, okay in the polynomial is much easier for similar reasons will also have the derivative to be much simpler.

Okay now we will look at case where we have derivatives from evenly space data, that is all the data points x_i plus 1 minus x_i are at equal distance that is all the x_i points are equal

distance and we call that distance as h. So h is the distance between any two data points this is evenly spaced data and we will do this thing with the specific example of a function f of x equal to e power to the x whose derivative we know very well.



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So we can, what we can do we can take this function and evaluate at some equal distance values and construct a difference table and then we will calculates the derivative from that and see what the error is etcetera like we did in the in the other newton's form earlier we will do the similar procedure here again.

So now in this case as I said that this difference table is little simpler at this x_1 minus x_0 equal to x_2 minus x_1 is equal to x_3 minus x_2 there is no need to keep those things here right. We need to differentiate that here, we have to divide that this thing, we can actually remove those points from here because we know that is a constant say irrespective of which point in that, we enter this is a constant we do not need to keep here and similarly, x_2 here minus x_0 , now two h we are going to write evenly spaced data we are going to say that x_i plus 1 minus x_i is equal to h that is what we are going to use all it becomes h this will become 2 h etcetera, so we do not need this also.

So as we can see the difference table will become simpler right and then to distinguish between this functions which we obtained from the newton's form for an equally distributed data to this, to distinguish between these two we change the notation here little bit call this as delta. Okay so we call it as this will become del 2 etcetera and this now delta, so that is a notation we would we use. So the next term this term will be two. Okay, so we have delta and we have del 2, then we have del 3 and we will continue with that okay so that is what would be that is a notation we are going to use and the difference table for the data which we obtained from this would look like following.

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Okay so now we have called delta del f_1 del square f del 3 f del 4 f del 5 f del 6 f etcetera as you so along. So notation we going to simply use f, okay that is what we will have okay I just del f here del 2 f here that is a function f itself, okay the derivative the difference in the function called delta f and the difference of the difference is called del square f etcetera, okay so that is the coefficients which we will have in this construction so this is just evaluated at equal distance that is h in this case point 6 as you can see, so "1.3" "1.9" etcetera and we evaluate the function which is e to the power of x, we know the functional form but let us say we do not know the functional form then we have some set of some data points given at that x values. (Refer Slide Time: 23:33)



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Then we construct the difference table just taking the difference between these two points as that here and the further differences, further differences that error represent as del n f. Okay so again this is, I put in here del f_i here, okay now this is again denote that which point on the difference table which we enter okay. So this is general notation, so if you enter as I said earlier that if we enter the difference table at 2 would be calling as delta f₂ del square f_2 , del 3 f_2 by del 4 f_2 etcetera if you enter a 3 and then we construct the polynomial this way, this way we will construct coefficient of the polynomial will go in this fashion. So that will be called del 3f del 3 square del 4 f, if you enter here this way it

will go that is the table will come back to the table again we need to look at this table when we actually do the example.

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1.1 f(x,M. $\Delta' f_i$ 3.669 -30 6.68 90 2.041 .672 2.50 12.182 1 386 1.118 3 058 3.10 22.198 2 504 5 562 15 004 3.70 40.447 12.333 27.337 4.30 73.700 60.590 4.90 134.290

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So the question what is the form of the polynomial now the form of the polynomial now this polynomial function we obviously have taken out the denominator from this point write as del f so del f is related to the coefficient of newton's form by saying that f of x_1 x_2 x_0 here f of x_1 x_0 will be del f of 1 del of 0 divided by h right we will have this kind of form f of x_1 or x_0 x_1 will be now del f we entered at this 0 divided by h that is what we have to divided by from the coefficient, so in general the formula is this we have to go

higher order terms, okay in general the formula is this seen earlier when you doing the polynomial interpolation that repeating those things here. So that is coefficient of the n th order term nth order term would be then del n f_i divided by n factorial into the h power of the n.

So again this point will be again the point this will be enter the data points, so del f_i is the difference between x_i plus 1 minus x_i , okay remember that x_i plus 1 minus x_i what is del f_i here, okay so now we will define a new variable called s, it is x minus x_i by h, now lets say we want to what we want to evaluate we want to evaluate the derivative all the polynomial at any point x.

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| Here Δf_i and is rela | is just the difference $f(x_{(i)}) - f(x_{(i)})$ ated to the coefficients of the interpolating |
|--|---|
| polynomia | al through $f[x_0, x_1, x_2, \dots, x_n] = \frac{\Delta^n f_i}{n! \hbar^n}$ |
| We will no | by define a variable $s = \frac{x - x_c}{h}$. |
| In this var | iable we can write |
| $(x - x_i)(x - x_i)($ | $(x - x_{i+1}) = (x - x_i)(x - x_i - h) = h^2 s(s-1)$ |
| similarly f | or other terms . |

So then, what is the now the terms the polynomial would be x minus x_0 x minus x_0 x minus x_1 etcetera right, that is what the polynomial was we had before, okay remember the polynomial newton's form was p_n of x would be written as we said f of x_0 , f of $x_0 x_1$ and the coefficient this is x minus x_0 other terms, okay now in the new notations would go just it as f of f x_0 plus now we have del here, del f right divided by h we said and then x minus x_0 okay plus other terms.

So now since, this is a h is a constant okay now we can define a new variable instead of writing x minus x_0 1x minus x_1 etcetera and we can define a new variable and that variable which we define as x minus x_0 by h because we entered here it as 0 this is del 0 del f_0 because we are entering 0 this is, so this is one way of writing.

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So we can define by x minus x_1 by h as variable, but in general if you enter any point here I, okay and we construct a polynomial from that okay now we will write the polynomial as n th order polynomial as we will say f_i at x₀ write that is the f x_i that is the value i enter lets some point x_2 here f x_2 and then we will have a del f₂ del f_i divided by h into x minus x_i as the first term and then we have a next term as remember del 2 f_i.

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Okay now you will have h square coming here okay because 2 h it will be h square into two that is what we will get coefficient okay and then we will get it as x square x minus

 x_i into x minus x_i plus 1 okay and will be other terms so then higher order term. So now what we have saying is that but x minus x_i plus 1 is we know that x_i plus 1 minus x_i is h, so we can write x_i plus 1 as x_i plus 1 now can be written as be as x plus x_i we can substitute that here. So you get x minus x i plus h okay, so we can write everything in terms of x minus x_i because all this are equal distance. So we can write everything in terms of x_i and to write down in a simple form, we define a new variable which is x minus x_i divided by h as s okay we defined as new variable x minus x_i divided by h as s which we saw in equal distance form in the polynomial interpolation and now with that we can write all the terms s for the example as I said x minus x_i plus 1 x_i plus 1 okay that would become x_i , x minus x_i we know is right now x_i plus 1 x_i plus h that is x_i plus 1.

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Here Δf_i is just the difference $f(x_{i,i}) - f(x_i)$ and is related to the coefficients of the interpolating polynomial through f[x]In this variable we can write $(x - x_i)(x - x_{i+1}) = (x - x_i)(x - x_i - h) = h^2 s(s - 1)$ similarly for other terms .

So I can write this is as x minus x_i into x minus x_i minus h that is if I define write in terms of variable we have h square into s minus 1. So advantage is when you notice that put it here in this coefficient okay in this coefficient multiplied by this coefficient these terms would get cancel and we only have a, n factorial in the denominator. Okay so in the form then we will have the polynomial which is of this form interpolating polynomial now simply have this particular form, so nth order polynomial were we enter at I write we enter I in the in the difference table so we have f of i s into del f_i plus s into s minus 1 by 2 factorial del f_i and s into s minus 1, s minus 2 by 3 factorial del three f_i etcetera, okay that is the advantage so when we have an equidistant points in the data points given are equidistant given then the whole thing simplifies to a polynomial of that form.

Okay so now the polynomial which we write would be will keep that in here the we will write the polynomial as p_n of x as f_i , so that is where we enter in to this 2 or 3 where we enter in the plus s into so we have s in to delta f_i plus s into s minus 1 by 2 into del 2 f_i plus s into s minus 2 divided by 3 into del 3 f_i .

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The interpolating polynomial is then $\prod (s-j) \frac{\Delta'' f}{r!} + error$

Okay that is the form we get you remember what del 1 f_i del 2 f_i given by s okay I to that start okay if you start from here if you start from here it is call two, you start from here i is 3 etcetera.

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Okay, the last term would be then a product of s minus j, j goes from 0 to n minus 1 del to the power n f by n factorial and then the next term is again the n plus 1 term is the error in the polynomial. Okay so now the derivative of this polynomial we can easily be written

once we have this form we can write the derivative remember s is the $x\mbox{ minus }x_i$ by h right.

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So the derivative with respect to x of this derivative with respect to x into ds by dx we will p d by dx of p_n of x as d by ds p_n of x into ds by dx. So then ds by dx over 1 h okay ds by d x_1 over h become 1 over h into d by ds of p_n of x and we know what is the derivative of that. So simply the reserved we will start with del f_i that will be the first term.

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Okay that is 1 over the h, so 1 over h into del f_i first term and the second term would be as you can see is the s minus 1 plus s right. So s minus 1 plus s by 2 the second term into del 2 f_i etcetera. So that is what we will get okay, so minus s plus 1 that is what I have written here the whole term I have written here okay. So the dx by ds give as 1 over h okay and the first term would be del f_i delta f_i and the second term would be s plus s minus 12 factorial into del f 2 i etcetera that is what we will get this is basically what we would have as a polynomial as a derivative. So now we can evaluate this derivative at any value x_1 once you given x we compute x then we can get the error is again derivative of the next term in the polynomial is the error in our function.

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The interpolating polynomial is then The derivative of this polynomial will then be time

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So we can apply this to specific problem where looking at the case that is where e to the power x. So we tabulated power to the x, so we can use the difference table look at particular example of this implementation of this again emphasize the point again i which we would use here okay a is the is to denote where we enter the difference table. Okay so now if you go back, let us say we want to evaluate the derivative at x equal to "3.9".

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| | \mathbf{x}_{i} | $f(\mathbf{x}_t)$ | M, | Δf_i | Δf_i | Δf_i | $\Delta^{i} f_{i}$ | $\Delta^{*}f_{i}$ |
|---|------------------|-------------------|--------|--------------|--------------|--------------|--------------------|-------------------|
| 0 | 1.30 | 3.669 | | | | | | |
| | 1 00 | | 3.017 | 2.479 | | | | |
| 1 | 1.90 | 0.000 | 5.496 | | 2.041 | 1 672 | | |
| 2 | 2.50 | 12.182 | 10.010 | 4.520 | 3,713 | 1.072 | 1.386 | |
| 3 | 3.10 | 22,198 | 10.010 | 8.233 | | 3.058 | | 1.118 |
| | | | 18.249 | | 6.771 | 5.562 | 2.004 | |
| 4 | 3.70 | 40.447 | 33.253 | 15.004 | 12.333 | | | |
| 5 | 4.30 | 73.700 | 60.590 | 27.337 | | | | |
| 6 | 4.90 | 134.290 | | | | | | |

So then x equal to "3.9", let us go back and look at the difference table okay we had the difference table here if you want to evaluate the derivative of the function "3.9". Okay so we could enter here 3.9 is between 4 and 5. So I could just enter here okay and then say that I will have the difference, I will construct a linear polynomial linear polynomial between 4 and 5. I have to enter at least 4, so the first thing I can do this that construct a linear polynomial between 4 and 5, okay that is saying that I will have only terms I have to do so in the derivative I will have the terms up to I have polynomial these two terms I am entering 4, so when I enter at 4 okay so I entered at 4. So I allow f of x_4 and f of x minus y f of x_4 the delta f_4 delta f_4 would be minus f of x_4 . So that is what would be and then x minus x_4 divided by h okay h in this case is ".6" that is what we will have so we can enter here.

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So and then construct my polynomial. So I can construct my polynomial the first term polynomial would "40.447" okay the next term would be "33.253" that is what the delta f $_i$ is into s what is s in this case is we want to construct 3.9". So s is if you want to do this in "3.9 " so at x equal to "3.9" s equal to 3.9 divided by minus x_i is "3.7" so it is ".2" divided by ".6" that is what we that is what we have s, okay we can construct that polynomial so if you note down this then is easy we that we enter here okay the first term in the "40.447" next term would be s into delta f i which is 1 by 3. So 1 by 3 into "33.253" that is our polynomial that is our linear polynomial.

So the linear polynomial is going to be in this particular case. So x "3.9" and we are entering at 4 x_4 is "3.7" okay, so s is 1 by 3 and the polynomial which we have order one polynomial would be f of x_4 so f of x_4 plus 1 by 3 into delta f_4 that returns out to be what we see here as "40.447" plus "33.25" 1 by 3 "33.253" that will be value evaluated p of x. Okay now everything here is number here, this is set to x equal to x equal to p at we can evaluate.

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A' fi A' fi N' fi $f(x_i)$ A S 1.30 3.669 3.017 2.479 6.686 1.90 2.041 5 4 9 1.672 2.50 12.182 1.386 10.016 1.118 3 0 5 8 3.10 22.198 2.504 6.77 5.562 15.004 3.70 40.447 12.333 1.527.337 4.30 73.700 60.590 4.90 134.290

So we do the polynomial or the p of x entering at we just f of x_4 "40447" plus s by s into "33.253" and the derivative of that polynomial which we know is 1 over h into dp by ds okay that is simply 1 over s by so 1 over h into "33.253" that is what we have so that is what we will get we will see that here.

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Okay so we could evaluated that etcetera "33.253" h is ".6" that is "33.256" by ".6". So that will be the error term what is the error in the term okay that is the next term in the polynomial as I said.

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Okay next term in the polynomial would be s into s minus 1 by 2 into del 2 f_i del 2 f_4 in this case okay that is the next term in the polynomial and so derivative of that would be s minus 1 plus 1 by 2 del 2 f_i into 1 over h okay that is the derivative that is the error, okay so we know that this value that is "33.253"

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by ".6" is not the correct derivative e to the power x e to the power 9 is not "33.253" is of by 7. So this is there is definitely approximately 7. So this definitely wrong because we just constructed a linear polynomial, so look at the error on this the error would be the next term in the polynomial and I said the next term in the polynomial. (Refer Slide Time: 41:41)

where the error term can be again evaluated using the next term rule of the interpolating polynomial. An important point to note: The index i used in the above expressions indicate the point at which we enter the difference table. For example: if we have to compute the derivative of $f(x) = e^t$ at x=3.9 using the above difference table we could enter at i=4 and use a polynomial of order one. This will result is the answer $\frac{d}{dx}P_2(x=3.9) =$ $\Delta f_4 =$ Error

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So far only taken this the next term would be that term, okay the derivative of that with respect is 1 over h 2 s minus 1 by 2 into del 2 f_i and we know all the thing, we know what del 2 f_i is so del 2 f_i is in the del 2 is del 24. So that is that is starting from four del two is "27.337" okay, so the error term, the error term which I called e is then 1 over h into 2 s minus 1 by so error here is 1 over h into 2 s minus 1 by 2 right that is what we

have 2 s minus 1 by 2 into del 2 f 4 okay that is the error in the term. Okay so del 24 is I am start from f 4 look at del 2, so starting from 4 is del 2 "27.337" and s we know 1 by 3.

So we can evaluate this this quantity, okay and write the error in that in this particular example case as "27.337" by ".6" that is 1 over h into s is to by 32 by 3 plus 2 by 3 minus 1 by 2 plus s minus 1 by 2.0kay so we can compare this will give something order "6.5" so we have very close to what the error which we expected to give.

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x-x, 3:9-3:7 The parameter x= and the error compare this is with the correct answer. Problem: Write a computer program to find the derivative of the function $f(x) = x \log(x)$ Construct the difference table using h=3 in the interval [x=1,x=4]. Evaluate the derivative and the error in the derivative at x=2.5 by using a 4th order polynomial. Enter the difference table at different points in the table, plot the error and derivative thus obtained against the value at which you entered the difference table.

So here is the another problem which you could look at then compare again by doing this evaluation, so notice that you can enter again in this particular example we had x_4 has because our data point which you want to get the derivative was between x_4 and x_5 . So we entered at x_4 constructed a linear polynomial and then we went to x_6 to construct the second order polynomial. So you could also do that by going backwards or you could go back x_3 , x_4 , x_5 and then construct a second order polynomial and then look at this error again okay that is compare that value the second order derivative we get from the second order polynomial by this form and entering making i as 3. Okay so we had 4 and then we went to then we went to 4, 5 and 6 points constructed this but we could make 3, 4 and 5.

Okay, so you have first enter at 4 i equal to 4 and use the linear polynomial and then enter at 3 construct a quadratic polynomial and then again compare the derivative and see what you get how much error you get.



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Okay so please note this function similar one and another function f of x log x okay and then you could again evaluate construct a difference table taking h as point 3 for example, and then between 1 and 4 you construct that difference table and write a program to do this and then use evaluate the derivative at x equal to "2.5" for example using polynomial of difference order and then look at look at the error in the polynomial.

Okay so going to the next part we are used to doing numerical differentiation we are used a formula called difference formula that is converting operator of this form d by dx of some function, okay into discrete this is continues form okay p_n of x is continuous function and then we can write d by dx is p_n of x. So when you have case of discrete evaluate at disserted points or you want to write a computer program to evaluate this thing okay one way is as you saw is to construct a polynomial and then takes the derivative okay or another way to do that to convert this function itself operated by d by dx itself in to a difference formula. Okay the two things you can do one is to say that I take my set of discrete points okay which I have a discrete data points I have okay I will make that into continuous function by getting a interpolating polynomial and I take the derivative of that function at any point I want and that is the best thing to do if you want to evaluate the derivatives at in between points, given as set of tabulated points you want to evaluate the derivative points in between the tabulated points and then you need to do something like this.

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Okay but suppose you want to evaluate the derivatives only at the tabulated points, okay then there is another method available that would be to say that I will write this, this whole operation derivative as itself as discrete operation.

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So I will make into discrete formula so I will not construct a polynomial but instead that I will just this into a discrete formula that is can be done only when we are evaluating this derivative at tabulated points okay that is d by dx of d by dx of f at x equal to x_i so if you want to evaluate the derivative of this function at any of this tabulated points okay then you could and also you do that okay by making this whole thing into a discrete formula, okay the whole process of taking the derivative into a discrete formula that is what we see here.

So we notice that the when we enter at any of the points which are tabulated then any of the points which are tabulated that is go back and look at whole form. We have the polynomial and s in terms of s, s is x minus xs by h. So now if you want to evaluate this polynomial at any of this tabulated points x_i okay then s could 0 because x minus x_i by h equal to 0 okay that is if I want to evaluate the derivative of this set of data points okay at least x 2 I want to find the derivative of this function at x_2 and I enter the difference table x_2 , okay and then s is 0 that is 0 I enter at x_0 and I want to evaluate the derivative x_2 . So p_n of x_i here could be s equal to 0 okay that is the point.

So the function here would simply would be simply p_n of x_i that is way we constructed that is obvious okay but then what will be the derivative that's is what question is what is p prime of x_i at x_i that would be x equal to 0 write s equal to 0 that will be 1 over h delta f_i plus minus del 2 f_i by 2 etcetera. Okay so we have not 0 terms in derivative this polynomial. So that is what one formula its one formula that gives one formula okay we just take this okay then I can write it in this form the full expansion will be like this. So what I have done want to evaluate the derivative, okay of the polynomial of the set of data points.

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Okay at some one of the tabulated points and I enter the difference table at that particular tabulated point and then I get s equal to 0 then I can write my derivative as 1 over h delta f_i minus del 2 f_i by 2 plus del 3 f_i by 3 etcetera up to minus 1. So we have alternatives 9 minus sign and we have minus 1 to the power minus 1 del n f_i by and the error again observes the order of next term would be of this form okay that will delta plus i plus 1. So looks at this in the case of second order derivative if I take this by a second order polynomial, okay at is physically say that terminate the set here and I take these two terms only okay what I would get delta f_i and then we have minus 1 by 2 del 2 f_i okay and del 2 f_i is delta $x_2 x_1$ minus delta $x_1 x_0$, so that is the further difference.

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Thus if we approximate the derivative by a second order polynomial the error is of third order and the derivative is OCh . This is known as the forward difference formulae for first derivative. In terms of the functions this is $[3f(x_i) - f(x_{i+1})] + O(h^2)$ equal to $\int (x_i)$ A more commonly used formulae for the first derivative is the one obtained from the polynomial of order one that is $f'(x_i)$ $\frac{1}{4} [f(x_{ex}) - f(x_{e})] + O(h),$

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So I can substitute for this in to this table okay, and then I would get okay f prime of x_i if I substitute for delta f_i , so let me write this here.

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| Thus if we app | roximate the derivative by a second |
|---------------------------------|--|
| be derivative i | ial the error is of third order and |
| lie derivative i | $\int f(\mathbf{x}_i) = \frac{1}{\mathbf{h}} \left[\Delta f_i - \frac{1}{2} \Delta f_i^{\dagger} \right] + O(\mathbf{h}^{\dagger})$ |
| This is known | as the forward difference formulae |
| or first derivat | ive. In terms of the functions this is |
| equal to $f'(x_i)$ | $=\frac{1}{2\hbar} \Big[4f(x_{i+1}) - 3f(x_i) - f(x_{i+1}) \Big] + O(\hbar^2$ |
| A more comr derivative is th | nonly used formulae for the first e one obtained from the polynomial |
| of order one th | at is $f'(x_i) = \frac{1}{h} [f(x_{i+1}) - f(x_i)] + O(h)$. |

So what I am saying is, I can write my derivative p_n of x_i using order 2 polynomial then I will get 1 over h into delta f_i minus del 2 f_i , del 2 f_i del 2 f_i by 2 is equal to 0, f equal to s equal to 0 by 2 what is delta f_i so we know delta f_i f of x_i plus 1 minus f of x_i del 2 f_i at I, f of plus 2 minus f of x_i plus 1 write minus f of x_i plus 1. Okay that is one term this is the difference of difference f of x_i that is what I get.

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Okay I can substitute into this equation okay and then I write p_2 prime of x into in to the form given here that is what given here. Okay I can substitute for del f_i , 2 del f_i and I will get it as 1 over 2 h plus 4 f of x_i plus 1 minus 3, f of x_i minus f of x_i plus 2 order of x square error in this okay so notice this thing, that here is the formula now given some x_i set of tabulated data points I want to find the derivative of the function at x_i , okay I could simply use this formula okay at this only involves points which are beyond x_i that is x_i if I want to find the derivative at x_i . I have to use the function value x_i plus 1 and x_i plus 2 okay at that this is called forward difference formula here is the forward difference formula what we normally known as okay which actually comes from this polynomial interpolation idea for equal difference points.

Okay say that if I want to evaluate the derivative of a function at given tabulated points then I can use I can use only two case three functions value above which is after $x_i x_i$ plus 1, x_i plus 2 okay and then I can write the formula as four f of x_i plus 1 minus 3, f of x_i minus f of x_i plus 2 by 2 h. Okay that is the formula which we can write, so now simpler formula which is commonly used is use a first order term just f of x_i plus 1 minus f of x_i divided by h as the derivative at that point. So now these are called difference formulas, okay we will use this actually solving the differential equations especially when you are doing the partial differential equation.

Okay we will convert the continuous differential equation in to a set of discrete equations we will allow to write down all over derivatives in a discrete form and that is what would be so now we can write this d f of x_i by dx, df by dx at x equal to x_i as discrete formula, okay something that which we can use in the in the thing okay.

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Thus if we approximate the derivative by a second order polynomial the error is of third order and the derivative is +0(h²) This is known as the forward difference formulae for first derivative. In terms of the functions this is equal to $f'(x_i) = \frac{1}{2\hbar} [4f(x_{i+1}) - 3f(x_i) - f(x_{i+1})] + O(\hbar^2)$ A more commonly used formulae for the first derivative is the one obtained from the polynomial of order one that is $f'(x_i) = \frac{1}{h} [f(x_{i+1}) - f(x_i)] + O(h)$.

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So now to evaluate the derivative x_i we can also do another thing that is to enter x_i minus 1 which I said we need not this formula which we obtained here by is by entering is to evaluate at x_i derivative at x_i by entering at i. Okay we could say I do not want to enter at i would enter at i minus 1, okay and then again use two terms so this will be delta f_i minus 1 del 2 f_i minus 1 by 2. I can do that okay and then, I can, then you will find do that i minus 1and then my x, my s, now okay, if I enter at I minus one okay. So if I take at i minus 1, so then s would be x minus x_i minus 1 right. So that is what we will have, okay x minus x_i minus 1 x_i divide by h that has to be 1.

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| To evaluate the | derivative at a if we can enter the |
|--|--|
| we will then have of order two will | $s = \frac{x_{j+1}}{s}$ and the derivative formulae |
| $f'(x_i) = \frac{1}{h} \left[\Delta f_{i,i} + \right]$ | $\frac{\Delta^2 f_{e1}}{2} + O(k^2) .$ |
| This is the cent derivative here is | ral difference formulae, since the $f(x_i) = \frac{1}{k} \left[\frac{f_{n1} - f_{k1}}{2} \right] + O(k^2)$ |
| Note that for evaluation this for forward difference We will now look | the same number of function ormulae is more accurate that the ce formulae. at higher order derivatives. |

So if you enter at i, s is 0 and if i enter at i minus 1, s is 1, okay so then if you do that okay s equal to 1, if i enter then will get my forward difference formula my difference formula sorry not forward difference formula is in a slightly different form. Okay I substitute for that here and then I will get my f prime of x_i as 1 over h f_i plus 1 my f of i minus 1 by 2, now this is another difference formula and this is known as symmetric difference formula, so we had a forward difference formula and we have a symmetric difference formula notice that here only two values of functions are used and we have

order h square accuracy while in the earlier case we had to get h square accuracy we had to use 3 values of the function 3 different values.

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Okay that is the difference between these two formulas but both of them order h square, okay we will look at, okay we will look at higher order derivatives in the using similar ideas in the next class.

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