

Numerical Methods and Computation
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Lecture No - 35

Numerical Differentiation and Integration (Continued)

Now in our previous lecture we have derived the numerical differentiation methods for a data which may be of non uniform mesh spacing or uniform mesh spacing. In particular way you use the Lagrange interpolation to derive the case of the non uniform mesh spacing and the Newton's forward difference formula for finding formulas for the uniform mesh spacing. Let us just briefly write down what are those formulas so that you can use them in some examples.

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Uniform Mesh Spacing
Quadratic Interpolation

$$f(x) \approx p(x) = f_0 + u \Delta f_0 + \frac{u(u-1)}{2!} \Delta^2 f_0$$

(i) $f'(x_0) = \frac{1}{2h} [-3f_0 + 4f_1 - f_2]$
 $E'(x_0) = \frac{1}{3} h^2 f'''(\xi), \quad x_0 < \xi < x_2$

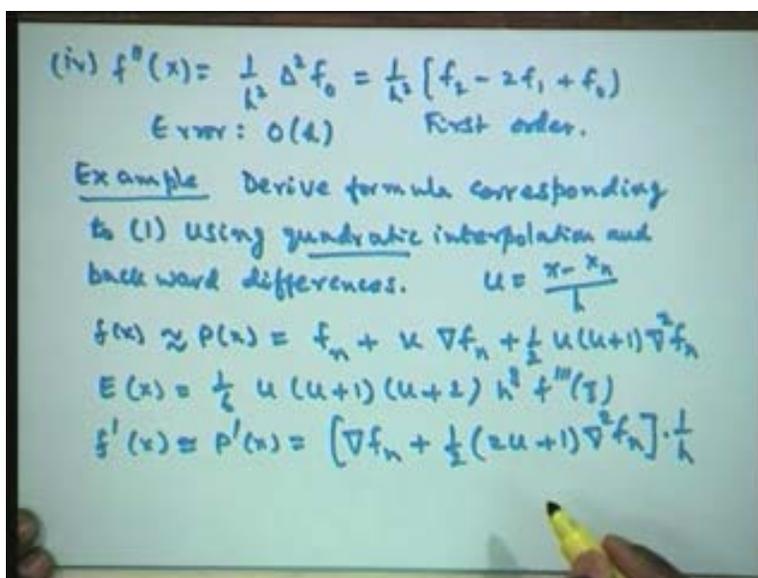
(ii) $f'(x_1) = \frac{1}{2h} [f_2 - f_0]; \quad E'(x_1) = -\frac{1}{6} h^2 f'''(\xi)$

(iii) $f'(x_2) = \frac{1}{2h} [3f_0 - 4f_1 + f_2]$
 $E'(x_2) = \frac{1}{3} h^2 f'''(\xi) \quad \text{Second order}$

So for the case of the uniform mesh spacing, uniform mesh spacing we have used the quadratic interpolation and linear interpolation also. Let us see what are the formulas that we got with quadratic interpolation. The starting point for which the Newton's forward difference formula, so we had written $f(x)$ is approximately $p(x)$ that is equal to f_0 plus u into Δf_0 plus $u(u-1)$ by factorial 2 into the second forward difference $\Delta^2 f_0$. Using this we have differentiated it and got the formulas for f' at x_0 is $\frac{1}{2h} [-3f_0 + 4f_1 - f_2]$

minus f_2]. The error for this was error at x_0 , we got it as h^2 by $3 f''$ triple dash of z , z lying between x_0 and x_2 . Is a quadratic interpolation so we are using only 3 points (x_0, f_0) , (x_1, f_1) , (x_2, f_2) . Now I can similarly find out the formulas for the first derivative at the middle point that is x_1 and this we derived it as 1 upon $2h$ as $[f_2 - f_0]$ and it is symmetrically placed, x_1 is symmetrically placed between x_0 and x_2 and the error in this case was, error at x_1 is equal to h^2 by $6 f''$ triple dash of z and the third formula that we can have at the last point that is f' dash at x_2 is equal to 1 upon $2h$ of $[3f_0 - 4f_1 + f_2]$, with the error being the same as earlier that this is equal to h^2 by $3 f''$ triple dash of z . So these are the formulas that we have derived last time, starting with the Newton's forward difference formula using upto second difference because it is only quadratic interpolation that we have obtained over here and we can see from here that this is a formula of order h^2 that means therefore it is a second order formula, this is also second order formula, this is also second order formula, all the formulas that we have written here is second order formulas. Now we can use the same formula to get the second derivative also.

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So if I can write down the fourth formula that we obtained was for second derivative f'' dash x , now since we started with quadratic interpolation that is a polynomial of degree 2 in u , the second derivative will give a constant therefore f'' double dash x was derived as a constant simply 1 upon h^2 delta square of f_0 . Therefore, and we have shown that the error is only of order h ; error is of order of h therefore this can be only a first order formula. Now to find the order it is not necessary that we should remember this particular formula, error formula and then derive it when once this formula is given to us, I can just use the Taylor expansions about the point that is given here, so this point here is x_0 so I can expand f_1 , f_1 means f at x_0 plus h , f_2 is f at x_0 plus $2h$, so 4 I can substitute this here, write the Taylor expansion of this, cancel all the terms, the leading term will be the term that is given here.

So we do not have to remember all this formula, I can use the Taylor expansions and get when ever required the order of the formula so they would all be the same thing. So let us just number it as 1, so that I want to use this in example. Now here again I can write down this, if I write this open it up and write 1 up on h square, this is forward difference $[f_2 - 2f_1 + f_0]$. I can Taylor expand it and show that it is of the first order, so let us take an example on this. So, now I will take a simple theoretical example first, derive formula corresponding to 1, corresponding to 1, I mean to say 1 is this particular formula that we have written here, we have numbered it as 1, Using quadratic interpolation and backward differences. Now as in the case of the interpolation here also a numerical differentiation, we need the formulas for the backward differences also the reason being if we are at the beginning of the data and we want the derivatives at any intermediate point or this, then I can use these formulas or this formula that I have written it writing $f'(x)$ here but if you are at the end of the table then forward differences are not available for us therefore I cannot use the forward differences. So when I want to find the derivative at a point at the end of the data, I need to have formulas using backward differences, therefore the starting point for this is again that we just write down the polynomial in terms of the backward differences.

So it will be f_n plus u backward difference with respect to Δf_n , this is half u into $(u + 1) \Delta^2 f_n$. So this is the formula that we have derived for the Newton's backward difference formula and the error for this was derived as $\frac{1}{6} u(u+1)(u+2) h^3 f'''(\xi)$. We have used it a quadratic interpolation, since its quadratic interpolation we have taken only upto the second backward difference and the error is of this particular form. Now I can differentiate this and write $f'(x)$ is equal to $p'(x)$, approximately $p'(x)$, the derivative is 0 so this is Δf_n , now plus I am using derivative with respect to u into $\Delta u \frac{du}{dx}$ that I will write it and this is equal to half u square that is $(2u + 1) \Delta^2 f_n$ into, you remember what is the formula for u, u was $x - x_n$ divided by h therefore $\frac{du}{dx}$ will be equal to $\frac{1}{h}$ here. Now this formula we shall use whenever we want to find the derivative at any arbitrary point at the end of the data x, we can find out when once x is given, I can find out the value of u from here, substitute it over and get the derivative. Even though this formula would get simplified, if I take the nodal point that is either x_n or $x_n - 1$ or $x_n - 2$, I can find formulas using at the nodal points. Now if I write the error, what will be the error at this point?

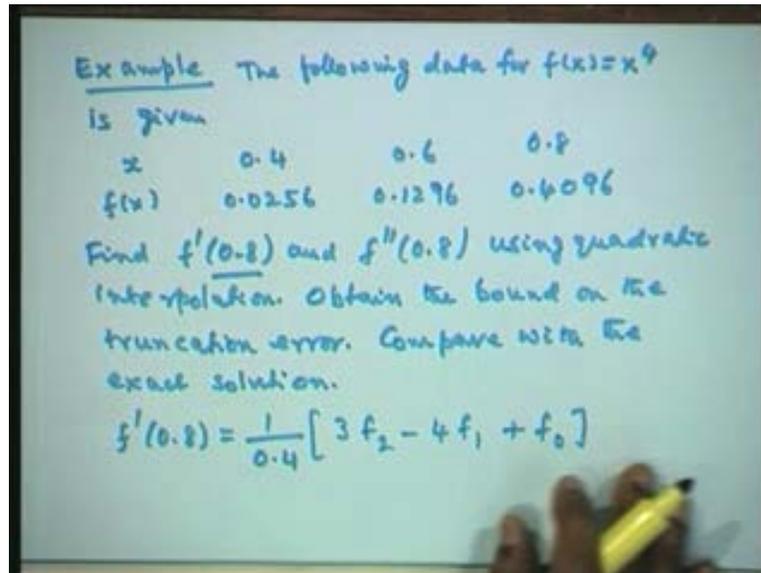
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$$\begin{aligned}
 E'(x) &= \frac{1}{6} \left[\frac{1}{h} \right] h^3 \left[\frac{d}{du} \{u(u+1)(u+2)\} f'''(\xi) \right. \\
 &\quad \left. + u(u+1)(u+2) \frac{d}{du} f'''(\xi) \right] \\
 &= \frac{h^2}{6} [\dots] \\
 \text{At } x=x_n, u=0 \\
 f'(x_n) &= \left[\nabla f_n + \frac{1}{2} \nabla^2 f_n \right] \cdot \frac{1}{h} \\
 &= \frac{1}{h} \left[(f_n - f_{n-1}) + \frac{1}{2} (f_n - 2f_{n-1} + f_{n-2}) \right] \\
 &= \frac{1}{2h} [3f_n - 4f_{n-1} + f_{n-2}] \\
 E'(x_n) &= \frac{h^2}{6} \cdot 2 \cdot f'''(\xi) = \frac{h^2}{3} f'''(\xi)
 \end{aligned}$$

I can differentiate this error, as error at x is 1 upon 6 , now again I am differentiating with respect to u and then 1 upon h so let us write down 1 upon h first that is du by dx , h cubed also let us write in first, then I differentiate this as a product so I will have d upon du $\{u$ into $(u$ plus $1)$ into $(u$ plus $2)\}$ into f triple dash of zhi plus u into $(u$ plus $1)$ into $(u$ plus $2)$ d upon du of f triple dash of zhi . Therefore in the general case this will look like h square by 6 into this quantity in the bracket. Now at the nodal points again this formula simplifies because we know at the nodal points this is going to be 0 . So let us derive at x is equal to x_n that is what we have been asked in the problem, derive the formula corresponding to formula 1 of this one. Now at x is equal to x_n , if I substitute it here I get u is equal to 0 so that means this is equal to u is equal to 0 .

Now therefore let us substitute u is equal to 0 in this, f dash at x_n is backward difference Δf_n plus u is equal to 0 so I will half $\Delta^2 f_n$ into 1 upon h . Let us simplify this, 1 upon h , this is $[(f_n$ minus $f_{n-1})$ plus half $(f_n$ minus $2 f_{n-1}$ plus $f_{n-2})$. Therefore this is 1 upon $2 h$, this is $2 f_n$ plus f_n $3 f_n$, minus $2 f_{n-1}$ minus $2 f_{n-1}$ minus $4 f_{n-1}$, plus I have f_{n-2} . This formula looks very similar to what we have here in the formula 1 expect that the suffixes have been changed and it is reversed. So we are, this formula is coming from this side, from x_0 inside whereas from this formula we are coming from x_n inside, in the opposite direction that is how the directions get changed here. Now let us find out what is the error at x dash at x_n . Now outside we have h square by 6 , so let us have this **h square**, u is equal to 0 therefore the second term goes off. Now I differentiate this as product of 3 terms, only 1 term will survive which will be the derivative of this particular part, derivative of this is this product, if you just put u is equal to 0 I will get a 2 , so I will get a 2 here and f triple dashed of zhi . So the error is again as we have in the previous case h square by $3 f$ triple dash of zhi . Okay let us actually take an example on this.

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The following data for $f(x)$ is equal to x to the power of 4, let us give the function also so that we can understand about the error, is given point 4, point 0 2 5 6, point 6, 1 2 9 6, point 8, 4 0 9 6. Find $f'(0.8)$ and $f''(0.8)$ using quadratic interpolation. Obtain the bound on the truncation error and since exact solution is given, let us compare with the exact solution also. Now we have asked to find derivative at point 8, point 8 is the last point of the data, therefore I need to use the backward differences that is the formula that we have just now derived. I must use this formula to find derivative at last point that means f' at 0 point 8 is 1 upon, the step length that is given to us is point 2, so that is 2 into h that is point 4, that is 3 times, let us write down the expression, this is, let us take f_0, f_1, f_2 , so this will be $[3f_2 - 4f_1 + f_0]$, $[3f_2 - 4f_1 + f_0]$, now let us substitute the values.

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x 0.4 0.6 0.8
 $f(x)$ 0.0256 0.1296 0.4096

Find $f'(0.8)$ and $f''(0.8)$ using quadratic interpolation. Obtain the bound on the truncation error. Compare with the exact solution.

$$f'(0.8) = \frac{1}{0.4} [3f_2 - 4f_1 + f_0]$$
$$= \frac{1}{0.4} [3(0.4096) - 4(0.1296) + 0.0256] = 1.84$$

So that is equal to 1 upon 0 point 4 [3 times (4 0 9 6) that is f_2 , 4 times f_1 (1 2 9 6) plus f_0 (0 point 0 2 5 6)] I can simplify this, the value is 1 point 8 4.

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Interpolation. Obtain the bound on the truncation error. Compare with the exact solution.

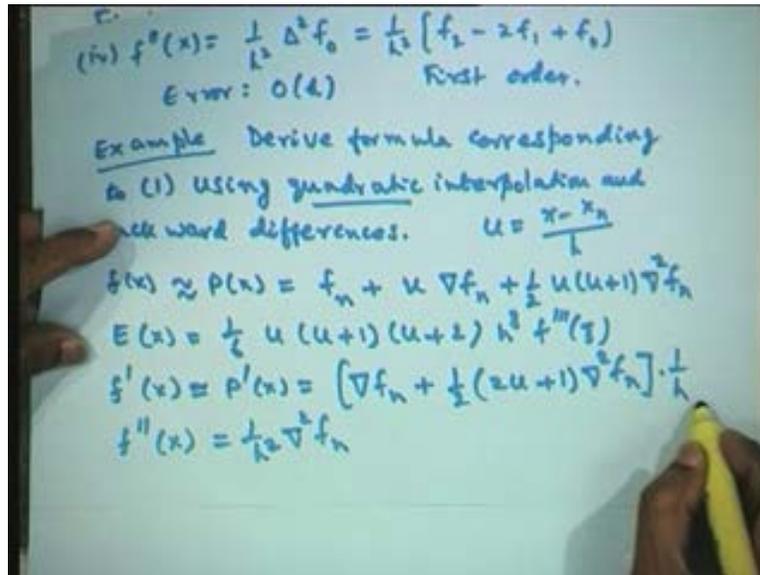
$$f''(0.8) = \frac{1}{(0.2)^2} \nabla^2 f_2$$
$$= \frac{1}{0.04} [f_2 - 2f_1 + f_0]$$
$$= \frac{1}{0.04} [0.4096 - 2(0.1296) + 0.0256] = 4.4$$

Exact. $f' = 4x^3$, $f'' = 12x^2$, $f''' = 24x$

$$f''(0.8) = 4(0.8)^2 = 2.048$$

Now I need the second derivative also, f'' (0 point 8). Now again from the previous formula, the previous formula that we have here is, we have written this, if I differentiate it once more f'' .

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Probably I could just write here and show this, that will become derivative of this will simply equal to $1 \text{ upon } h \text{ delta square } f_n$ into h , $1 \text{ upon } h$, therefore $1 \text{ upon } h$. I am differentiating respect to u therefore du by dx will also come $1 \text{ upon } h$, $1 \text{ upon } h \text{ square delta square } f_n$ which corresponds to the formula in the forward difference, $1 \text{ upon } h \text{ square forward difference formula at } 0$. Therefore what I have here is $1 \text{ upon } h \text{ square that is } 1 \text{ upon } 2 \text{ whole squared}$, our step length is point 2 and this is your delta square of f_2 , you will have here $0 \text{ delta square of } f_2$. Therefore I can write this as $1 \text{ upon } 0 \text{ point } 0 \text{ 4 delta squared } f_2$ that is equal to, backward difference so I will have $[f_2 \text{ minus } 2 f_1 \text{ plus } f_0]$. So let us substitute these values $1 \text{ upon } 0 \text{ point } 0$, f_2 is the last value **4 0 9 6** minus 2 times the middle value **1 2 9 6** plus f_0 is $0 \text{ point } 0 \text{ 2 5 6}$. Now I can find out its value it comes out to be $4 \text{ point } 4$.

Now let us first of all see what is the error by using the exact solution, the exact solution is f'' , let us differentiate it that is $4 x \text{ cubed}$ and for second derivative f'' is $12 x \text{ square}$ and we need for the error also, let us write down the third derivative that is equal to $24 x$. Therefore the exact solution is f'' at (point 8) that is (point 8) whole cubed. I have the value here that is $2 \text{ point } 0 \text{ 4 8}$.

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The image shows a whiteboard with handwritten mathematical work. At the top, there is a partially visible equation: $= \frac{1}{0.4} [3(0.4096) - 4(0.1296) + 0.0256] = 1.84$. Below this, a more complete equation is written: $= \frac{1}{0.04} [f_2 - 2f_1 + f_0]$. This is followed by a numerical calculation: $= \frac{1}{0.04} [0.4096 - 2(0.1296) + 0.0256] = 1.84$. Below this, the function and its derivatives are defined: Ex. 11.4. $f' = 4x^3$, $f'' = 12x^2$, $f''' = 24x$. Then, the first derivative is evaluated at $x=0.8$: $f'(0.8) = 4(0.8)^3 = 2.048$. The error is calculated as $\text{Error} = 2.048 - 1.84 = 0.208 \checkmark$. Next, the second derivative is evaluated at $x=0.8$: $f''(0.8) = 12(0.8)^2 = 7.68$. The error is calculated as $\text{Error} = 7.68 - 4.4 = 3.28 \checkmark$.

Now let us, before we find the second derivative let us now find out what is the error. The error is 2 point 0 4 8 that is the exact solution minus 1 point 8 4 is the solution which we have got here, so this is equal to this, subtract 1 point 8 4 therefore you have got here point, **0 point 0 2 8, 0 point 2 8** is the error, it is quite large error, let us see why it is happening, we can find it out. Now let us find the exact solution, second derivative f_2 that is 12 into (point 8) whole square. This is 7 point 6 8. The error in this case is the exact solution 7 point 6 8 minus the numerical solution that we have got minus 4 point 4, therefore the error is 3 point 2 8, these are the actual errors in the problem. Now let us see what our theoretical values of the error tell us, now the theoretical expression for the first derivative error is h^2 by 3 $f'''(z)$, therefore let us try to find out the error from this.

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$$|E'(0.8)| \leq \frac{h^2}{3} M_3 ; \quad M_3 = \max_{[0.4, 0.8]} f'''(x)$$

$$M_3 = \max_{[0.4, 0.8]} 24x = 24(0.8) = 19.2$$

$$|E'(0.8)| \leq \frac{0.04}{3} (19.2) = \underline{0.256}$$

$$|E''(0.8)| \leq h M_3$$

$$= 0.2 (19.2) = \underline{3.84}$$

$$f'(0.7) \quad u = \frac{x - x_n}{h} = \frac{0.7 - 0.8}{0.2}$$

$$= -\frac{0.1}{0.2} = -0.5$$

Therefore the magnitude of the error at point 8 is less than or equal to, I am writing from here h^2 square by 3 M_3 , M_3 is the maximum of $f'''(x)$ in the given interval, the given interval is [point 4, point 8], so in this interval. Now we have found out the third derivative is $24x$ so I can find out what is M_3 , M_3 is maximum of within the interval 0 to point 8, the third derivative is $24x$. Therefore this is 24 into point 8 that is equal to 19.2 . So it is because of this reason our actual error is large and our numerical value also shows that it is the, error is going to be large because M_3 is very very large. So let us write down, substitute it here, therefore derivative, error at the derivative is point h^2 is 0.04 divided by 3 into 19.2 that is 0.256 .

Now you can see that the actual error is point 0.208 and theoretically it is predicted that error is going to be point 0.256 , so the actual error would always be less than this because this is the maximum possible error in the problem. Now let us derive the expression for the error in the second derivative, h^2 is less than or equal to h upon h into M_3 and this is equal to point 2 , so this gives us 3.84 . Now this is the error that is predicted and the actual error is 3.28 so again the actual error is less than the predicted error. Therefore we given a data and the point at which we want the derivative, a first derivative or the second derivative, if it is at the beginning of the data we shall use the forward differences, if you are at the end of the data we shall use the backward differences and using this formula we could have computed not necessarily the solution at point 8, we could have find the numerical solution at any intermediate point also but then we shall be using the original formula that we started with. For example, if I want to find what will be the derivative at point 7, I shall be using this value by finding what will be the u .

For example if you are asking for what will be the value at f' at point 7 then I will be using, finding out my value of u , u is equal to x minus x_n by h and here x_n the last point is point 8 and step length that is given in the problem is point 2, so this will be minus point 1 by point 2 that is 1 by 2 that is minus point 4. Therefore u , the value of u would be minus point 5 and I shall be using this value of u in this expression to find out what will be the value of the derivative at a non-mesh point, so any point; intermediate in the point. So I shall use this formula directly by finding u and substituting over here, same thing is true for the derivatives also. The formulas that we have derived so far can also be derived alternatively by using the difference operators.

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2. Difference operation
 $E, \Delta, \nabla, \delta$
 $E = 1 + \Delta, E = (1 - \nabla)^{-1}, \delta = E^{1/2} - E^{-1/2}$
 $\delta = \frac{d}{dx}$
 $E f(x) = f(x+h)$
 $= f(x) + h D f + \frac{h^2}{2!} D^2 f + \dots$
 $= [1 + h D + \frac{h^2 D^2}{2!} + \dots] f(x)$
 $= e^{hD} f(x)$
 $E = e^{hD}; hD = \log E$

If you remember that we have derived the difference operators, the difference operators, we have defined mainly the operators E the shift operator, forward difference, backward difference, central difference. We just need the definitions to derive this formulas, E is equal to 1 plus delta, E is also equal to $(1 \text{ minus backward delta})^{-1}$ and delta is E to the power of half minus E to the power of minus half, these are the relations that we have derived between these operators. Now we have also derived the relationship between the dy by dx derivative operators and these operators, let us just relook in to that particular aspect. If I write down E of $f(x)$ which gives me the shift by 1 unit that is f of $(x \text{ plus } h)$, let us write the Taylor series of this, so this gives $f(x)$ plus h , now I will use the D for d by dx , I will write down notation D for d by dx therefore instead of f' , I will write down D of f x h square by factorial 2, second derivative that is D of d , d square of $f(x)$ and so on. So this is my Taylor series. I will now write this as $[1 \text{ plus } h D, h \text{ square } D \text{ square by factorial 2 and so on}]$ operate on $f(x)$. So I have taken the **operate**, the $f(x)$ on to the right, so that I operate on $f(x)$ this particular operator and this symbolically I can write this as exponential of $h D$ operate on $f(x)$.

So if I open up exponential of hD will have $1 + hD$, h^2 , h^3 whole square by factorial 2 h^3 cube factorial 3 and so on. So whatever is there in the bracket is the symbolic expansion of exponential of hD . Therefore the operator E must be equivalent to the operator exponential of hD , therefore the operator E is equivalent to exponential of hD or if I take logarithm on both sides hD is equal to \log of E . Now it is this would, that would give us the formulas that we have derived here, so my starting point is here.

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The whiteboard contains the following handwritten text:

$$hD = \log E$$

$$= \log(1 + \Delta) = \Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \dots \quad (2)$$

$$= \log(1 - \nabla)^{-1}$$

$$= -\log(1 - \nabla) = \nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \dots \quad (3)$$

$$hD f(x) = \left(\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \dots \right) f(x) \quad (4)$$

$$= \left(\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \dots \right) f(x) \quad (5)$$

One term: first order $O(h)$
 Two terms: second order $O(h^2)$

So I take hD is equal to \log of E but E is $1 + \Delta$, if I want the forward, in terms of forward differences I will substitute E is equal to $1 + \Delta$, so I will write this as \log of $1 + \Delta$. Then symbolically open up logarithm, this will be $\Delta - \Delta^2/2 + \Delta^3/3$ and so on. We have numbered earlier 1, let us number it as 2. Now if want backward differences, I will now use E is equal to $1 - \nabla$ inverse, so I will write this as \log of $1 - \nabla$ inverse. Let us take minus 1 out so this will be minus of \log of $1 - \nabla$. Now let us expand this logarithm, this will be minus $\Delta - \Delta^2/2 + \Delta^3/3$ and so on. That means if you operate it on any given function $f(x)$, now that will be simply either I have Δ , $\Delta^2/2$, $\Delta^3/3$ and so on operate on $f(x)$ or I will have this as backward ∇ , $\nabla^2/2$, $\nabla^3/3$ and so on operate on $f(x)$. Now I can get the formulas by just cutting the series at 1 term, I can cut it after 2 terms; I can get it after 3 terms and so on, so all the formulas that we obtained earlier can also be obtained from here. If I use only 1 term in this expansion, I will get first order formulas that means order of h formulas I will get. If I use 2 terms that means I am using up to Δ^2 here and backward difference square by 2 then I will get all second order formulas, order of h^2 square formulas.

Whatever we have derived earlier using the forward or the backward differences or obtained using this particular formula also but there was 1 formula earlier which we have derived at the point, middle point which we have shown it as symmetrically placed f_2 minus f_0 by $2h$. Now let us have a look at how that formula can be obtained and for that I will use the central difference, this particular formula, the formula that we have written.

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$$\begin{aligned} \delta &= E^{h/2} - E^{-h/2} = e^{hD/2} - e^{-hD/2} \\ &= 2 \sinh\left(\frac{hD}{2}\right) \\ hD &= 2 \sinh^{-1}\left(\frac{\delta}{2}\right) \\ &= 2 \left[\left(\frac{\delta}{2}\right) - \frac{1}{6!} \left(\frac{\delta}{2}\right)^3 + \dots \right] \\ &= \delta - \frac{1}{24} \delta^3 + \dots \quad (6) \end{aligned}$$

We have delta is equal to E to the power of half minus E minus half but E is equal to exponential of hD , so I will write down exponential of hD by 2 minus exponential of minus hD by 2. Now this is of the form some exponential of x minus exponential of minus x that is equal to 2 sine hyperbolic x , so I can write this as 2 times sine hyperbolic hD by 2. Now I can bring 2 to the left hand side and invert this to find hD therefore hD is equal to, let us take 2 also to the right, 2 times sine hyperbolic inverse delta by 2. We bring 2 to the denominator, invert it, sine hyperbolic inverse hD is equal to 2 sine hyperbolic delta by 2.

Now the expansion of sine hyperbolic, the first two terms is same as sine inverse, the first two terms of sine hyperbolic inverse is also same as first two terms of sine inverse. So let us write down those 2 terms, that is sine inverse is, sine inverse x is x minus x cubed by factorial 3 so that will be delta by 2 minus 1 upon factorial 3 into delta by 2 whole cubed. The first 2 terms will be the same that means I can write this as delta minus 1 upon 24 delta cubed, this is 8 into 6 48 we have multiplicative factor here so on. So this is the derivative, first derivative in terms of the central difference. Now if I want the second derivatives, the second derivatives is almost trivial because what we are looking for is D square, so if hD gives me this, I can operate pre multiply by hD therefore h square D square will be operator square, operator square.

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Two terms: second order

$$= 2 \sinh\left(\frac{hD}{2}\right)$$

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

$$= 2 \left[\left(\frac{\delta}{2}\right) - \frac{1}{3!} \left(\frac{\delta}{2}\right)^3 + \dots \right]$$

$$= \delta - \frac{1}{24} \delta^3 + \dots \quad (6)$$

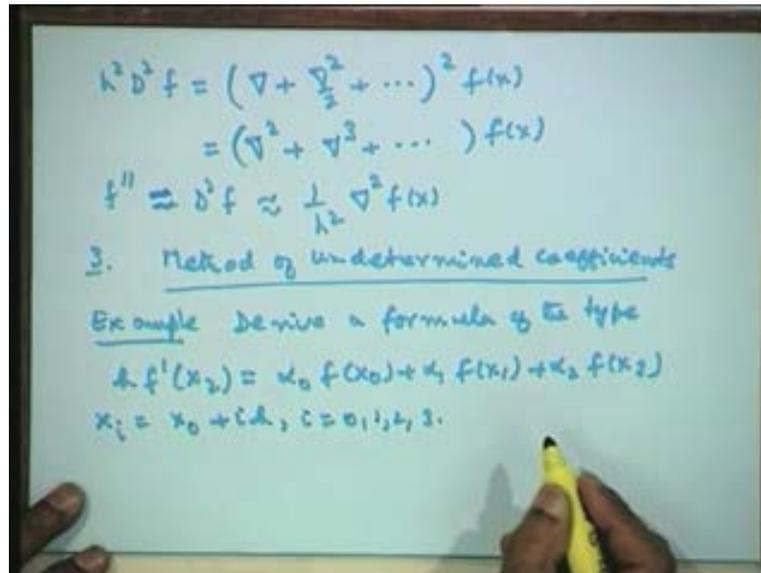
$$h^2 D^2 = \left(\delta - \frac{\delta^3}{24} + \dots \right)^2$$

$$= \delta^2 - \delta^4 + \dots$$

$$f'' = D^2 f \approx \frac{1}{h^2} \delta^2 f$$

Therefore if I want the second derivative, I just have to operate on the left by hD here therefore it will be simply the square of this, delta, delta square by 2, delta cubed by 3 so on whole square. So I just have to take the square of this that will give me the, hD operator is being pre multiplied once more so I will simply have this square of this operator as this one that means this will be, let us open it up delta squared, the product of this is delta cubed, I am writing the first 2 terms, delta square 2 times this 1 that is minus delta cubed plus so on. Now you can see again, if I cut the first term what we have done earlier we get it that is D square is approximately 1 upon h square delta square. This is what we have derived earlier using the forward differences that second derivative D square, this is your second derivative f double dash, put f here, put f here, so second derivative is simply 1 up on h square delta squared f and if I write one more term, I will be using more number of points. Now I can use similarly the backward differences just as I have done it to here, I can use the back ward differences this,

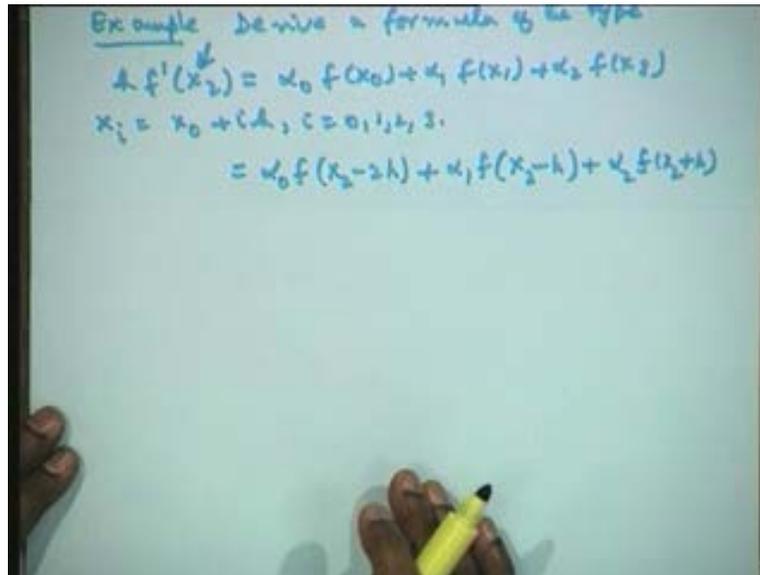
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h square D square of f will be square of this backward difference, delta square by 2 whole square of f(x). Therefore this will be delta square plus delta cubed so on of f(x). Now again whatever we have done earlier we can get here, the second derivative approximation is D squared of f, this is D squared of f; this is approximately 1 upon h square delta square of f(x). So this was a formula we have derived f double dash at x_n is 1 upon h square delta squared of f(x), so we have got the same formulas again. I can therefore use the next term also, next term is delta cubed so I will be using more number of points to get the formula over here. Therefore the formulas that we have obtained using the interpolation can be obtained by using the difference operators also without any change what so ever. Now let us see what will happen in the third case that we said method of undetermined coefficients, method of undetermined.

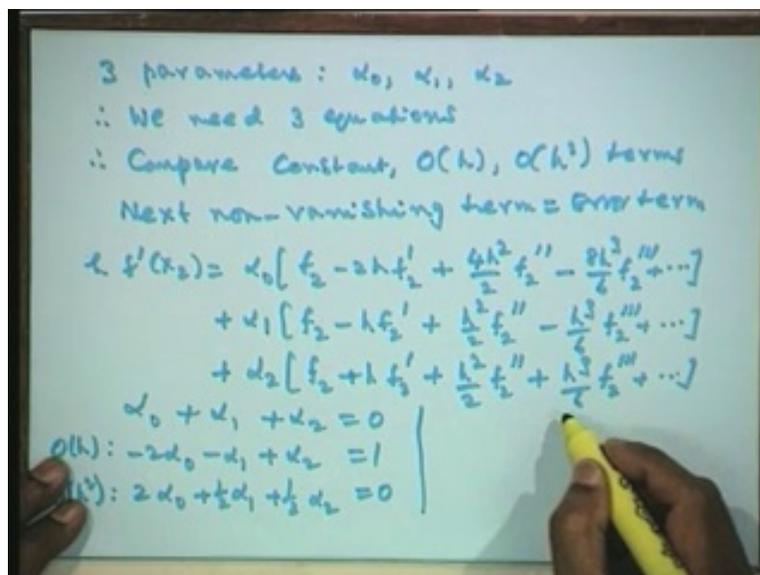
In this case the method that you want depending on the data that is given to us, data is given randomly so if you are given a data, you would like to use only those data points in construction of the formula and let us assume that such formula is not available for you either through difference operators or through the interpolation, then what we do is we just write down the formula that we want, use the Taylor expansions, compare the coefficients and find out the parameter that are involved there. So that is a very simple and straight forward procedure so I will illustrate it through an example. Let us take it as an example, now derive a formula of the type $h f'(x_2)$ is $\alpha_0 f(x_0)$, $\alpha_1 f(x_1)$, $\alpha_2 f(x_2)$, $f(x_3)$, where x_i is equal to x_0 plus $i h$, i is equal to 0, 1, 2, 3. As I said the solution for this is very straight forward, I need the expansion of this about the point that we have been asked on the left hand side, the point we have been asked is x_2 on the left hand side, therefore I will write this as $\alpha_0 f(x_2 - 2h)$.

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x_0 is 2 units behind x_2 therefore x_2 minus 2h, $\alpha_1 f$ of x_1 is 1 unit behind x_2 that is your (x_2 minus h) and the third term is x_3 is 1 unit ahead of x_2 so this will be f of (x_2 plus h). Now I have here 3 parameters $\alpha_0, \alpha_1, \alpha_2$, therefore I need 3 equations to determine them therefore I write the Taylor expansion and compare the constant h, h square term.

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Because there are 3 parameters, there are 3 parameters to be determined α_0 , α_1 , α_2 therefore we need 3 equations, we need 3 equations therefore compare the constant term, order of h , order of h square terms, order of h square terms. The next non vanishing term is the error, so the error is the next non vanishing term, is the error term; is the error term. Now I will write down only 1 step and leave it as example for you. So if I now write this, open it up, what I would get here is $\alpha_0 f(x_2)$ lets write down suffix 2, minus $2 h f''(x_2)$ plus $2 h^2$ whole square that is $4 h^2$ square by factorial 2 f_2'''' double dash, I need error term so I will write down the next one also, minus $8 h^3$ cubed by $6 f_2'''$ triple dash at 2, this is the expansion of the first term. The second term is $\alpha_1 f(x_2)$ minus $h f_2''$ dash plus h^2 square by $2 f_2''''$ double dash minus h^3 cubed by $6 f_2'''$ triple dashed and so on. And the third term is α_2 is x_2 plus h therefore f_2 plus h times f_2' prime h^2 square by $2 f_2''$ double prime plus h^3 cubed by $6 f_2'''$ triple prime and so on.

Now I need to compare the constant, there is no constant on the left hand side that is 0 therefore α_0 , α_1 , plus α_2 will be 0, α_0 , α_1 plus α_2 is equal to 0. Now we compare order of h terms. On the left hand side we have 1, $h f'$ dash coefficient is 1 so let us write down 1. On the right hand side $h f_2'$ dash is minus $2 \alpha_0$ minus α_1 plus α_2 , so I have minus $2 \alpha_0$ minus α_1 plus α_2 . Then we compare order of h square, there is no h square on the left hand side therefore have the right hand side as 0. Here, we have got here h^2 square f_2'' double dash 4 by 2 that is $2 \alpha_0$; this is half α_1 half α_2 so I have got here $2 \alpha_0$ plus half α_1 plus half α_2 . Now I can solve this for α_0 , α_1 , α_2 , it is determined. Now if you look at the error now, the error would be, now the next non vanishing term, the next term is the minus 4 by $3 \alpha_0$ minus 1 by $6 \alpha_1$ plus 1 by $6 \alpha_2$ into h^3 cubed f_2''' triple dashed so we can substitute the values of α_0 , α_1 , α_2 in that and then write down that this is the error in this particular formula. Therefore given any particular formula which is required in a particular application, one can use the Taylor expansions determine the parameters that are there and then find out the error expression also. Now we have been a commenting in the last lecture that the numerical differentiation could be an unstable process and the reason is that the round off errors can seriously effect this computation. What do we mean by this let us just see, let us say, what is the effect of round off errors? And the other error that is truncation errors, the effect of round off and truncation errors.

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Effect of Round off and Truncation errors

$$f''(x_0) \approx \frac{1}{h^2} [f(x_2) - 2f(x_1) + f(x_0)]$$

$$T.E = \frac{1}{2} f''(\xi), \quad x_0 < \xi < x_2$$

$$f''(x_0) = \frac{1}{h^2} [f(x_2) - 2f(x_1) + f(x_0)] + hf'''(\xi)$$

Round off error: $\epsilon_0, \epsilon_1, \epsilon_2$ in f_0, f_1, f_2
 $\pm 5 \times 10^{-4} \quad \pm 1 \times 10^{-4}$

$$f''(x_0) = \frac{1}{h^2} [(f_2 + \epsilon_2) - 2(f_1 + \epsilon_1) + (f_0 + \epsilon_0)] + TE$$

$$= \frac{1}{h^2} [f_2 - 2f_1 + f_0] + RE + TE$$

$$RE = \frac{1}{h^2} (\epsilon_2 - 2\epsilon_1 + \epsilon_0)$$

Now I shall illustrate it through an example, as I have done in the previous case, let us take any particular formula, let us take the formula that we have derived using the forward differences this, this is approximately 1 upon h square $[f(x_2)$ minus twice $f(x_1)$ plus $f(x_0)]$. Now we are given the error expression for this already so let us take this error for this as truncation error is equal to h f'''' of ξ , ξ lying between x_0 and x_2 . As I said given a formula we do not have to remember what is your truncation error, we just write down the Taylor expansions of these terms about the point that is given here that is your x_0 , so I can open it up, cancel of all the terms and then whatever the leading term of the error will be my truncation error so that is my truncation error. Now if I add the truncation error, I should get the, here I put an approximately it will become exact, so I add the truncation error to it, whatever error is there I add it to it, I will get the exact solution that means f'' at x_0 is equal to 1 upon h square f of x_2 minus twice f of x_1 plus f of x_0 plus the truncation error h f'''' of ξ .

Now let us assume that there is round off error, so let us say there is round off errors; let us take $\epsilon_0, \epsilon_1, \epsilon_2$ the round off errors in f_0, f_1, f_2 . Of course if it is a data that is given to us then if the entire data is accurate to 4 decimal places or 6 decimal places correspondingly ϵ will be, say if it is 4 places we may say that its error is 1 into 10 to the power of minus 4 or if you are using round off then you can say 5 into 10 to power of minus 4. So we will be able to tell, it will be plus minus, will be able to say what is the round off error in a given table of values when once we are said that you have got a 4 plus accuracy, 6 plus accuracy and so on. So we know these expressions but alternatively we can have also that the errors in each one of them could be different also.

So let us take the general case when the errors are this one, therefore in actual computation it is not $f(x_2)$ that is being computed but $f(x_2)$ plus ϵ_2 is the error. Therefore we are actually getting here in computations is 1 upon h square $[(f_2 \text{ plus } \epsilon_2) \text{ minus } 2 \text{ times } (f_1 \text{ plus } \epsilon_1) \text{ plus } (f_0 \text{ plus } \epsilon_0)]$ plus, let us write down this as TE for truncation error. Therefore this is equal to 1 upon h square $[f_2 \text{ minus } 2 f_1 \text{ plus } f_0]$, now I will write this as round off error plus truncation error. Where the round off error is whatever is corresponding to round off error that means round off error is 1 upon h square $(\epsilon_2 \text{ minus twice } \epsilon_1 \text{ plus } \epsilon_0)$. So I collected the terms from here, 1 upon h square ϵ_2 minus 2 ϵ_1 and this, and the truncation error is we have here. Now you can see, let us find out what is the magnitude of this round off error.

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Handwritten mathematical derivations on a whiteboard:

$$|R.E| \leq \frac{1}{h^2} [|\epsilon_2| + 2|\epsilon_1| + |\epsilon_0|]$$

$$\leq \frac{4E}{h^2} \quad E = \max |\epsilon_i|$$

$$|T.E| \leq h M_3, \quad M_3 = \max |f'''(x)|$$

$$|T.E| \rightarrow 0 \text{ as } h \rightarrow 0$$

$$|R.E| \rightarrow \infty \text{ as } h \rightarrow 0$$

$$E = 1 \times 10^{-4} \quad \frac{4 \times 10^{-4}}{h^2}$$

So the magnitude of this round off error is less than or equal to 1 upon h square [magnitude of ϵ_2 twice magnitude of ϵ_1 plus magnitude of ϵ_0]. If you call this epsilon as the largest of all this, I will just have this, this I can simply write this as 2, 3, 4, 4 times epsilon by h square and what is the magnitude of truncation error? The truncation error is h into, I think I have written it wrong, it is f triple dash, this truncation error is h f triple dash zhi therefore this will be h into M_3 , M_3 is the maximum of f triple dash of x . Now you can see why we were so much worried of the round off errors, if you look at this quantity, this round off error is being divided by this step length h square whereas truncation error we are multiplying by h . Now if in a, what we mean by convergence we are speaking of, we are saying that if we have given a table of values with the step lengths say point 5, if I reduce the step length by a factor then it will be much more accurate that means as h tends to 0 if you take smaller and smaller step length for constructing a table then it will be more and more accurate.

It is true because truncation error would always tend to 0 as h tends to 0 because this is always going to 0, therefore truncation is always going to 0 therefore if you use smaller and smaller step length; yes we are going to get better accuracy but if there is round off error in the problem what would happen? As h tends to 0 round off error can blow up because we are dividing by h , h square, we know what is our epsilon which may be 10^{-4} or 10^{-5} by h square but this is where the whole difficulty is, this tends to infinity as h tends to 0. You see for example, if you are taking say epsilon is 10^{-4} then if you are taking this epsilon as 10^{-4} , this would imply this is 10^{-4} divided by h square depending on the step length. Now you can see that if h is smaller and smaller going to point 0, this is going to be very big quantity and therefore the round off error can blow up and it can really **play havoc in** finding the numerical solution and hence we say this numerical differentiation can be an unstable process. Now we are going to analyze this further and give concretely the quantity or what is the total error that we are committing in a, in any particular problem, given a formula we shall be able to say exactly what would be the error in terms of epsilon and how it is going to behave, that we shall take it in the next class.