

Scientific Computing Using Matlab
Professor. Vivek Aggarwal and Professor. Mani Mehra
Department of Mathematics
Indian Institute of Technology, Delhi

Lecture - 54

Higher Order Accurate Numerical Differentiation Formula for Second Order Derivative

Hello viewers, welcome back to the course on Scientific Computing in Matlab. So, we will continue with the Numerical Differentiation, as we have discussed in the previous lecture. So, in the previous lecture, we have discussed how we can find out the first order derivative; whenever data is given to us that is not equispaced. And we are able to find this expression number 3 for that one.

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Lecture-54

Second order derivative I

Using eq. ① & ②, we eliminate $f'(x_0)$.

Multiply ① by $(x_1 + x_2)$ and eq. ② by x_1 and subtract.

$$(x_1 + x_2)f_1 - x_1 f_2 = \left[f(x_0) - f'(x_0)x_1 + \frac{f''(x_0)x_1^2}{2!} - \frac{f'''(x_0)x_1^3}{3!} + \dots \right] (x_1 + x_2) - \left[f(x_0) - f'(x_0)x_1 + \frac{f''(x_0)x_1^2}{2!} - \frac{f'''(x_0)x_1^3}{3!} + \dots \right] x_1$$

$$\Rightarrow (x_1 + x_2)f_1 - x_1 f_2 - x_1 f_0 = \frac{x_1(x_1 + x_2)}{2} f''(x_0) + \frac{x_1^3(x_1 + x_2)}{6} f'''(x_0) + \dots$$

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Lecture-54

Second order derivative I

Using eq. ① & ②, we eliminate $f'(x_0)$ from eq.

Derivation with unequal intervals!

$x_0 \quad x_1 \quad x_2 \quad \dots \quad x_n$
 $y_0 \quad y_1 \quad y_2 \quad \dots \quad y_n$

$x_1 = x_0 + h_1$
 $x_2 = x_0 + h_1 + h_2$

Taylor's expansion
 $f(x_0 + h_1) = f(x_0) + h_1 f'(x_0) + \frac{h_1^2}{2!} f''(x_0) + \dots$ (1)
 $f(x_0 + h_1 + h_2) = f(x_0) + (h_1 + h_2) f'(x_0) + \frac{(h_1 + h_2)^2}{2!} f''(x_0) + \dots$ (2)

1st order derivative
 sub. eq. (1)

$f'(x_0) = \frac{f(x_1) - f(x_0)}{h_1} - \frac{h_2}{2} f''(x_0)$

$f'(x_0) = \frac{f(x_1) - f(x_0)}{h_1} + O(h_1)$

$h_i = x_{i+1} - x_i$

NPTEL

Derivation with unequal intervals!

$x_0 \quad x_1 \quad x_2 \quad \dots \quad x_n$
 $y_0 \quad y_1 \quad y_2 \quad \dots \quad y_n$

$x_1 = x_0 + h_1$
 $x_2 = x_0 + h_1 + h_2$

Taylor's expansion
 $f(x_0 + h_1) = f(x_0) + h_1 f'(x_0) + \frac{h_1^2}{2!} f''(x_0) + \dots$ (1)
 $f(x_0 + h_1 + h_2) = f(x_0) + (h_1 + h_2) f'(x_0) + \frac{(h_1 + h_2)^2}{2!} f''(x_0) + \dots$ (2)

1st order derivative
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$f'(x_0) = \frac{f(x_1) - f(x_0)}{h_1} - \frac{h_2}{2} f''(x_0)$

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$h_i = x_{i+1} - x_i$

NPTEL

Now today, I want to find out that how we can approximate the second order derivative. Now, we will use the expression 1 and 2 as we have discussed. So, using equation 1 and 2; so that is given to me. So, this is the equation number 1, and this is the equation number 2. We eliminate $f'(x_0)$ from equation. Using this one, we eliminate $f'(x_0)$. So, let us eliminate this one. So, how we can eliminate, multiply equation number by $h_1 + h_2$ and equation 2 by h_1 and subtract.

So, let us see what will happen. Now what I am doing, I am multiplying this one, because I want to remove this. So, I multiply this by $h_1 + h_2$ and this one by h_1 and then I subtract. So, let us see what will happen. So, I will get the expression $(h_1 + h_2)f_1 - h_1 f_2$. So, this I am getting, because this is my f_1 , and this is my f_2 . So, I am getting $(h_1 + h_2) f_1$; h_1 , and this is

$h_1 + h_2$ minus h_1 x naught. So, this is $(h_1 + h_2 - h_1)f_0$. So, that is what I am getting. Then this one, h_1 multiplied by $h_1 + h_2$ and this is a $h_1 + h_2$ multiplied by h_1 . So, this will

cancel out. And the next expression, I will get, is $(h_1 + h_2) \frac{h_1^2}{2!}$. So, this is I am getting

$\frac{-h_1(h_1 + h_2)^2}{2!}$. And this I am getting a second derivative at x naught. So, this is the second derivative I am getting at x naught. Now that the third one is the next one is, it will be

plus $(h_1 + h_2) \frac{h_1^3}{3!} - h_1 \frac{(h_1 + h_2)^3}{3!}$. This is my third derivative and so on. So, this I am getting. Now from here, this will cancel out. Now from here, I can write that this expression becomes $(h_1 + h_2)f_1 - h_1f_2 - h_2f_0$. Now from here, let us see that,

what the common term we can take. So, if you see from here, I can take $\frac{h_1(h_1 + h_2)}{2}$. So, this one 2 factorial is 2, so this is just 2 value. If I had taken common from here; so I will get here $h_1 - (h_1 + h_2)$, this one. Now from here, the same way, I will get the terms $h_1(h_1 + h_2)/6$. So, inside I will get $h_1^2 - (h_1^2 + h_2^2)$; because this will come out $f'''(x_0)$ and so on.

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Handwritten mathematical derivation on a digital whiteboard:

$$\Rightarrow \frac{(h_1 + h_2)f_1 - h_1f_2 - h_2f_0}{2} = -f''(x_0) + \frac{h_1(h_1 + h_2)}{6} f'''(x_0)$$

$$\Rightarrow f''(x_0) = \frac{2(h_2f_0 + h_1f_2 - (h_1 + h_2)f_1)}{h_1h_2(h_1 + h_2)} - \frac{h_1(h_1 + h_2)}{3h_2} f'''(x_0)$$

$x_0 \leq x \leq x_2$

$f''(x_0)$ is of $O\left(\frac{h_1 + h_2}{2}\right)$

Let us choose $h_1 = h_2 = h$

$$f''(x_0) = \frac{2(h_2f_0 + h_1f_2 - 2h_1f_1)}{h^2 \cdot 2h} = \frac{f_0 - 2f_1 + f_2}{h^2}$$

Cancel order derivative operation

Now, from here I can write this expression, and this will cancel out and I will get $-h^2$. So from here, I can write this expression as

$$\frac{(h_1 + h_2)f_1 - h_1 f_2 - h_2 f_0}{\frac{h_1 h_2 (h_1 + h_2)}{2}} = -f''(x_0) + \frac{h_1(h_1 + h_2)(h_1^2 - h_2^2 - h_2^2 - 2h_1 h_2)}{6 \frac{h_1 h_2 (h_1 + h_2)}{2}} f'''(x_0) + \dots$$

; because I am taking the common terms, so I will divide the term, all the terms after this. So from here, my second order derivative,

$$f''(x_0) = \frac{2(h_2 f_0 + h_1 f_2 - (h_1 + h_2)f_1)}{h_1 h_2 (h_1 + h_2)} - \frac{h_2(h_2 + 2h_1)}{3h_2} f'''(\xi) \quad x_0 \leq \xi \leq x_2$$

. So, this will cancel out and from here, I get this expression. So now from here, I can say that my second order derivative at x_0 is of this form. That contains the value at x_0 at x_2 and x_1 and this is of order h^2 . So, this formula is of order h^2 , using the third order derivative, Now let us see, what will happen. So, let us choose $h_1 = h_2 = h$.

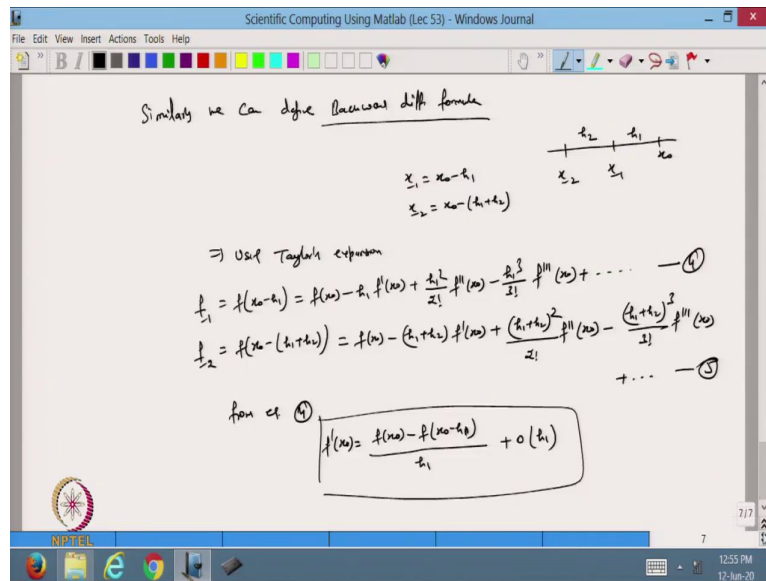
So let us see, what will happen, in that case, it will be second derivative at x_0 . This is h , this is h , it is $2h$. So, I can take this common; so I will get $2h$ so inside I will get

$$\frac{f_0 - 2f_1 + f_2}{h^2} \quad . \text{ And this is my second order derivative. So, using the central scheme.}$$

$$\frac{f_0 - 2f_1 + f_2}{h^2}$$

So, this is a central second order derivative. That is $\frac{f_0 - 2f_1 + f_2}{h^2}$. So, this is the central second order derivative, difference scheme, operator. So, that we can define. And now if we put h and h here, so this will be of order h in this case. But generally, it is of order h^2 , so that is when we do the expression that will come out. So, this is the way we can, we are able to write the second order derivative for un-equispaced data.

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Now, this is, we have used for the forward; similarly, we can define backward difference formula. So, in the backward difference formula; suppose, we have the un-equispace data. And let it is my x_0 , this is my x_1 and this is my x_2 . This is my h_1 and this my h_2 . Or you can take as, $x_i, x_{i-1}; x_{i-2}$. Does not matter. So, I can write from here, this is my

$$x_{-1} = x_0 - h_1 \text{ and this is } x_{-2} = x_0 - (h_1 + h_2).$$

So from here, now using Taylor's expansion, we can define the function at, so this I define as f at minus 1.

$$f_{-1} = f(x_0 - h_1) = f(x_0) - h_1 f'(x_0) + \frac{h_1^2}{2!} f''(x_0) - \frac{h_1^3}{3!} f'''(x_0) + \dots$$

So, this terms we can take, so I just define this as equation number 3, so it is 4. Let us take it 4. Similarly,

$$f_{-2} = f(x_0 - (h_1 + h_2)) = f(x_0) - (h_1 + h_2) f'(x_0) + \frac{(h_1 + h_2)^2}{2!} f''(x_0) - \frac{(h_1 + h_2)^3}{3!} f'''(x_0) + \dots$$

. So, this is equation number 5. Now from here, if I take the first order derivative. So, from equation, from equation number 4, we can find the simple first order derivative. So, I can

$$f'(x_0) = \frac{f(x_0) - f(x_0 - h_1)}{h_1} + O(h_1)$$

define this as . So, this is the backward difference operator for the first order derivative. So, that we already know, if $h_1 = h$ then this

is just the backward operator for the equispaced data. So, this one we can define very easily then.

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higher order 1st derivative

from eq. (2), put $-h_1, h_2$ instead of h_1, h_2

we get

$$f'(x_0) = \frac{h_1^2 f_2 - (h_1 + h_2)^2 f_1 + h_2^2 f_0}{h_1 h_2 (h_1 + h_2)} + \frac{h_1 (h_1 + h_2)}{6} f'''(\xi)$$

$x_0 \leq \xi \leq x_2$

Similarly, we can derive second order derivative

$$f''(x_0) = \frac{2}{h_1 h_2 (h_1 + h_2)} \left\{ h_2 f_0 - (h_1 + h_2) f_1 + h_1 f_2 \right\} + \frac{1}{2 h_2} \left\{ (h_1 + h_2)^2 - h_1^2 \right\} f''(\xi)$$

$x_0 \leq \xi \leq x_2$

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$$\Rightarrow f'(x_0) = \frac{(h_1 + h_2)^2 f_1 - h_1^2 f_2 - (h_1 + h_2)^2 f_0}{h_1 h_2 (h_1 + h_2)} + \frac{(h_1 + h_2) h_1}{6} f'''(\xi)$$

$x_0 \leq \xi \leq x_2$

$f'(x_0)$ is of order $O((h_1 + h_2) h_1)$

if $h_1 = h_2 = h$

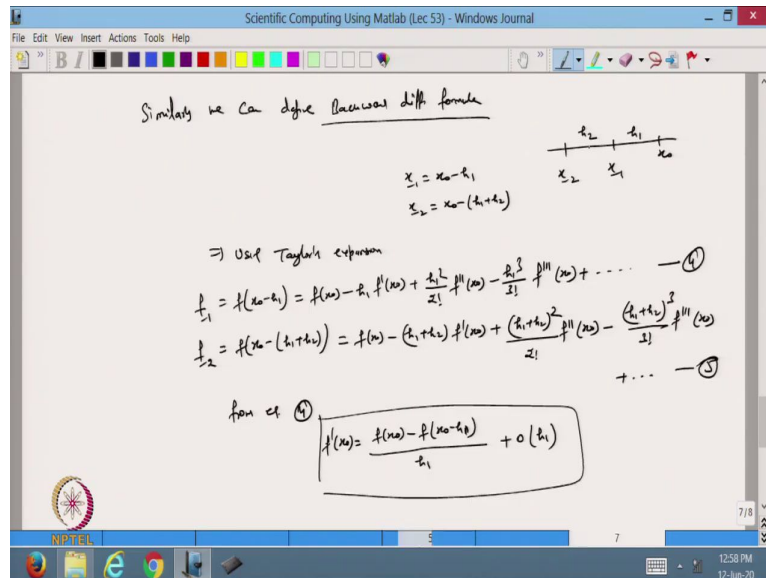
from eq. (3), we get

$$f'(x_0) = \frac{(2h)^2 f_1 - h^2 f_2 - (2h)^2 f_0}{2h \times h^2} + \frac{(2h) h}{6} f'''(\xi)$$

$$= \frac{4f_1 - f_2 - 3f_0}{2h} + \frac{h^2 - h^2}{6} f'''(\xi)$$

$4f_1 - f_2 - 3f_0$

$h^2 - h^2 = 0$



Now suppose, I want to define this for the higher order derivative. So, higher order first derivative. So, the same way we have done in the previous lectures, this one. So, if I take this expression, for the first derivative from equation number 3 and instead of h_1 and h_2 I put $-h_1$ and $-h_2$. So, let us take a, from equation 3 putting $-h_1$ and $-h_2$, instead of h_1 and h_2 . So, we get, so, if I do that one, so this will be the same, square term is there. This is also square, this is also square, but here it will be $-h_1 - h_2$ and this is a minus sign here.

So now, if I just write that one, then our f' at x_0 can be written as,

$$f'(x_0) = \frac{h_1^2 f_{-2} - (h_1 + h_2)^2 f_{-1} + h_2^2 f_0}{h_1 h_2 (h_1 + h_2)} + \frac{h_1 (h_1 + h_2)}{6} f'''(\xi) \quad x_{-2} \leq \xi \leq x_0$$

. Actually, if you see in this case, this h_1 and h_2 was this one; it was my x_0 , x_1 and x_2 . So, it was my h_1 and this my h_2 . Now, I have x_0 , x_{-1} and x_{-2} . So, this is, I am writing as h_1 and h_2 ; just to write the same expression, but otherwise you can also write this as a h_0 or h_1 , so does not matter. But we are going forward.

So, that is the expression for the first order derivative, using the backward. Similarly, because the same expression I have to do again and again, similarly we can derive second order derivative. So, in the second order derivative, I do the same thing. I have the 3 values; 1, 2, and 3. So 3 points stencil is there, and if I do this one, I can eliminate the value of f' at x_0 . So, I can write this directly. So, this will come out,

$$f''(x_0) = \frac{2}{h_1 h_2 (h_1 + h_2)} \{h_2 f_0 - (h_1 + h_2) f_{-1} + h_1 f_{-2}\} + \frac{1}{3h_2} \{(h_1 + h_2)^2 - h_1^2\} f'''(\xi)$$

, where ξ is belonging from this one.

So, from here I can write directly, but this expression you can find by eliminating the f' from this expression. So I want to, if I want to eliminate this f' from here and from here, I will multiply by h_1 and plus h_2 here, and by h_1 and then I subtract. So, this will cancel out and then we can derive this formula. So, we will get this formula for the second derivative. So, this is the formula for the second derivative.

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Central diff formula

Use Taylor's expansion

Diagram: $x_0-h \quad x_0 \quad x_0+h$

$$h_1^2 f'(x_0) = f(x_0+h_1) - f(x_0) + \frac{h_1^2}{2!} f''(x_0) + \dots \quad (6)$$

$$h_2^2 f'(x_0) = f(x_0-h_2) - f(x_0) + \frac{h_2^2}{2!} f''(x_0) - \frac{h_2^3}{3!} f'''(x_0) + \dots \quad (7)$$

To find first order derivative

$$h_1^2 \times (6) - h_2^2 \times (7)$$

$$h_1^2 f_1 - h_2^2 f_{-1} = (h_1^2 - h_2^2) f_0 + (h_1^2 h_2^2 + h_2^2 h_1^2) f''(x_0) + \dots$$

$$\Rightarrow \frac{h_1^2 f_1 - h_2^2 f_{-1} - (h_1^2 - h_2^2) f_0}{h_1 h_2 (h_1 + h_2)} = f'(x_0) + \frac{h_1^2 h_2^2 (h_1 + h_2)}{6 \times 2! (h_1 h_2)} f'''(\xi)$$

Now what will happen, if I want to define the central difference formula. Till now, we were heading either on the right-hand side, means forward or the backward. Now, what will happen if I have x naught here and this is my x_0+h and this is my x_0-h . And I will call it this h_1 and I call it this h_2 . So basically, this is my f_1 , this is my f_0 and this is my f_{-1} .

Now in this case, I want to go forward also and backward also. So, we will go one point forward and one point backward. So that is the way, we can define the central difference formula. So in this case, I know that using Taylor's expansion, I have to take x_0+h_1 plus so on. So this I, 4, 5, 6, I will take it as equation number 6. And then I will take x_0-h_2 , going backward. So, if you see this one, then it will be

$f(x_0 - h_2) = f(x_0) - h_2 f'(x_0) + \frac{h_2^2}{2!} f''(x_0) - \frac{h_2^3}{3!} f'''(x_0) + \dots$. So, I call it equation number 7. So, in this case I am going forward and backward also.

Now, to find out the first order derivative, what I will do, now to approximate, to find the first order derivative. The finite difference formula for first order derivative. So, what I will do is that; in that case, I want to find these values. So, what I do, I will eliminate, suppose I will eliminate f' , second derivative. So, what I will do that, I will multiply this by h_2 square, and I multiply this by h_1 square, and then subtract. So, h_2 square multiply equation 6 minus h_1 square multiply equation number 5. So, what we will get, we will get

$$h_2^2 f_1 - h_1^2 f_{-1} = (h_2^2 - h_1^2) f_0 + (h_1 h_1^2 + h_1^2 h_2) f'(x_0) + \left(h_2^2 \frac{h_1^3}{3!} + h_1^2 \frac{h_2^3}{3!} \right) f'''(x_0) + \dots$$

. Now, from here I can write this expression as

$$\frac{h_2^2 f_1 - h_1^2 f_{-1} - (h_2^2 - h_1^2) f_0}{h_1 h_2 (h_1 + h_2)} = f'(x_0) + \frac{h_2^2 h_1^2 (h_1 + h_2)}{6 h_1 h_2 (h_1 + h_2)} f'''(\xi) ; \text{ all}$$

other terms are ignored.

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$$\Rightarrow f'(x_0) = \frac{h_2^2 f_1 - h_1^2 f_{-1} - (h_2^2 - h_1^2) f_0}{h_1 h_2 (h_1 + h_2)} + O\left(\frac{h_1^2}{h_2^2}\right)$$

if $h_1 = h_2 = h$

$$f'(x_0) = \frac{f_1 - f_{-1}}{2h^2} + O\left(\frac{h^2}{6}\right)$$

$$f'(x_0) = \frac{f_1 - f_{-1}}{2h} + O(h^2)$$

Central diff formula:
 Use Taylor's expansion

$$h_2^2 f_1 = f(x_0) + h_1 f'(x_0) + \frac{h_1^2}{2!} f''(x_0) + \dots \quad (1)$$

$$h_1^2 f_{-1} = f(x_0) - h_2 f'(x_0) + \frac{h_2^2}{2!} f''(x_0) - \frac{h_2^3}{3!} f'''(x_0) + \dots \quad (2)$$

To find first order derivative

$$h_2^2 \times (1) - h_1^2 \times (2)$$

$$h_2^2 f_1 - h_1^2 f_{-1} = (h_2^2 - h_1^2) f(x_0) + (h_1 h_2^2 + h_1^2 h_2) f'(x_0) + \left(\frac{h_2^2 h_1^2}{2!} + \frac{h_1^2 h_2^2}{2!} \right) f''(x_0) + \dots$$

$$\Rightarrow \frac{h_2^2 f_1 - h_1^2 f_{-1} - (h_2^2 - h_1^2) f(x_0)}{h_1 h_2 (h_1 + h_2)} = f'(x_0) + \frac{h_1^2 h_2^2 (h_1 + h_2)}{6 \times h_1 h_2 (h_1 + h_2)} f'''(x_0)$$

So, from here this will cancel out, this will also cancel out. So, I can write my central finite difference for first order derivative, for the first order derivative. So, this becomes

$$f'(x_0) = \frac{h_2^2 f_1 - h_1^2 f_{-1} - (h_2^2 - h_1^2) f_0}{h_1 h_2 (h_1 + h_2)} + \mathcal{O}\left(\frac{h_1 h_2}{6}\right)$$

So, that is

the expression, central difference expression for the first order derivative for un-equispaced data.

Now this one I can write, if $h_1 = h_2 = h$; then for equispaced data I can write this as, so h and h I can take common. So, this will be 0. In that case, I can write from here,

$$f'(x_0) = \frac{h^2 (f_1 - f_{-1})}{2h^3} + \mathcal{O}\left(\frac{h^2}{6}\right)$$

Now this will, I cancel out, and from here I

will get

$$f'(x_0) = \frac{(f_1 - f_{-1})}{2h} + \mathcal{O}(h^2)$$

And this is I know, that this is the first order centre scheme for the first order derivative. So, that is the way we can verify this one.

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2nd order derivative!

eliminate $f(x_0)$ from eq ⑥ & ⑦

$$h_2 f_1 + h_1 f_{-1} = (h_1 + h_2) f_0 + \left(\frac{h_2 h_1^2}{2!} + \frac{h_1 h_2^2}{2!} \right) f''(x_0) + \left(\frac{h_2 h_1^3}{3!} + \frac{h_1 h_2^3}{3!} \right) f'''(x_0) + \dots$$

$$f''(x_0) = \frac{h_2 f_1 - (h_1 + h_2) f_0 + h_1 f_{-1}}{\frac{h_1 h_2}{2} (h_1 + h_2)} - \frac{(h_1 - h_2) f'''(x_0)}{6 \frac{h_1^2 + h_2^2}{(h_1 + h_2)}}$$

if we choose $h_1 = h_2 = h$

Central diff formula

Use Taylor's expansion

$$h_2^2 f_1 = f(x_0) + h_1 f'(x_0) + \frac{h_1^2}{2!} f''(x_0) + \dots \quad \text{⑥}$$

$$h_1^2 f_{-1} = f(x_0) - h_2 f'(x_0) + \frac{h_2^2}{2!} f''(x_0) - \frac{h_2^3}{3!} f'''(x_0) + \dots \quad \text{⑦}$$

To find first order derivative

$$h_2^2 f_1 - h_1^2 f_{-1} = (h_2^2 - h_1^2) f_0 + (h_1 h_2^2 + h_1^2 h_2) f'(x_0) + \left(\frac{h_2^2 h_1^3}{3!} + \frac{h_1^2 h_2^3}{3!} \right) f'''(x_0) + \dots$$

$$\Rightarrow \frac{h_2^2 f_1 - h_1^2 f_{-1} - (h_2^2 - h_1^2) f_0}{h_1 h_2 (h_1 + h_2)} = f'(x_0) + \frac{h_2^2 h_1^2 (h_1 + h_2)}{6 \times \frac{h_1^2 h_2^2}{(h_1 + h_2)}} f'''(x_0)$$

Now, I can give one more expression for a second order derivative. So, second order derivative. So, I can eliminate, so from 6 and 7 eliminate $f'(x_0)$, from equation 6 and 7. So, we can eliminate that one. So how can we eliminate it? I want to eliminate the first order this one. So, I will multiply this by h_2 and this by h_1 , and then we will add. So in that case, if I do that one, then I can write

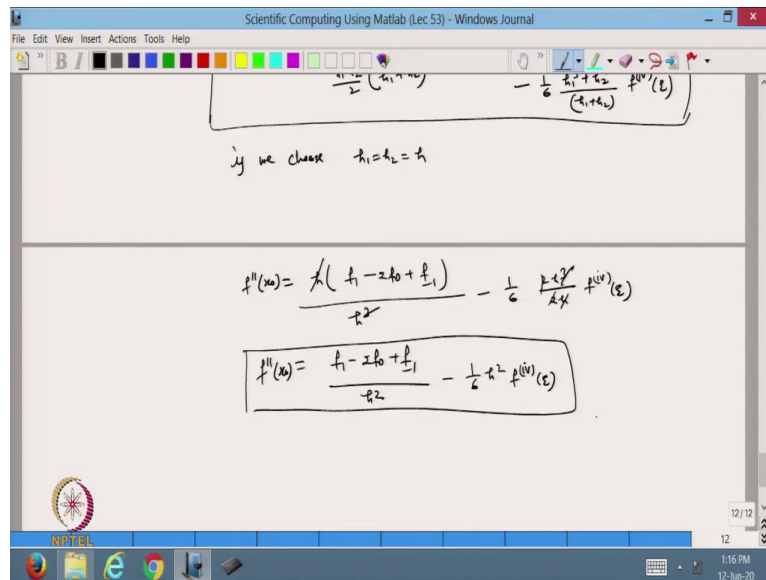
$$h_2 f_1 + h_1 f_{-1} = (h_1 + h_2) f_0 + \left(h_2 \frac{h_1^2}{2!} + h_1 \frac{h_2^2}{2!} \right) f''(x_0) + \left(h_2 \frac{h_1^3}{3!} + h_1 \frac{h_2^3}{3!} \right) f'''(x_0) + \dots$$

. Now, I can take my h_1 and h_2 on the left-hand side, taking this term together. So from here, I can write directly that my

$$f''(x_0) = \frac{h_2 f_1 - (h_1 + h_2) f_0 + h_1 f_{-1}}{\frac{h_1 h_2}{2} (h_1 + h_2)} - (h_1 - h_2) f'''(x_0) - \frac{1}{6} \frac{h_1^3 + h_2^3}{(h_1 + h_2)} f^{(iv)}(\xi)$$

. So, this will be the expression for second order derivative using the centre scheme. And now, from here you can verify that if we choose $h_1=h_2=h$.

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Then my $f''(x_0)$ can be written as. So this will be h , this will be $2h$, this will be h . So, I can write my h common. So, this will be

$$f''(x_0) = \frac{h(f_1 - 2f_0 + f_{-1})}{h^3} - \frac{1}{6} \frac{2h^3}{2h} f^{(iv)}(\xi)$$

. So this will cancel out, and this will cancel out. So from here, I can write that this is equal to

$$f''(x_0) = \frac{(f_1 - 2f_0 + f_{-1})}{h^2} - \frac{1}{6} h^2 f^{(iv)}(\xi)$$

. And that we already know, that if we have the equispaced data and we want to find out the second order finite difference, using the central scheme. So, this is the expression for that one and that is of order h^2 . So, this one we can verify by putting $h_1=h_2=h$.

So let me stop here. So, today we have discussed that how we can derive the formulas for the first order derivative, for the second order derivative, of higher accuracy that is of order h or order h^2 using for the data that is not equispaced. And with this one, we will want to

close this unit that is a numerical differentiation. And from the next lecture, we will continue with the next unit that is numerical integration. So, I hope that you have enjoyed this one. Thanks for watching, thanks very much.