

Homework #4

<1> 4th order central difference (1st derivative)

Given equations are :-

$$(a) f(x+2\Delta x) = f(x) + 2\Delta x f'(x) + 2\Delta x^2 f''(x) + \frac{4}{3} \Delta x^3 f'''(x) + \frac{2}{3} \Delta x^4 f^{(4)}(x) + O(\Delta x^5)$$

$$(b) f(x-2\Delta x) = f(x) - 2\Delta x f'(x) + 2\Delta x^2 f''(x) - \frac{4}{3} \Delta x^3 f'''(x) + \frac{2}{3} \Delta x^4 f^{(4)}(x) + O(\Delta x^5)$$

$$(c) f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{1}{2} \Delta x^2 f''(x) + \frac{1}{6} \Delta x^3 f'''(x) + \frac{1}{24} \Delta x^4 f^{(4)}(x) + O(\Delta x^5)$$

$$(d) f(x-\Delta x) = f(x) - \Delta x f'(x) + \frac{1}{2} \Delta x^2 f''(x) - \frac{1}{6} \Delta x^3 f'''(x) + \frac{1}{24} \Delta x^4 f^{(4)}(x) + O(\Delta x^5)$$

We want to zero out columns 1, 3, 4 and 5 and sum the coefficients of column 2 to 1. Suppose columns 1, 3 & 5 can be zeroed out using $(\tilde{a}, -\tilde{a}, \tilde{b}$ and $-\tilde{b})$, which leaves us with columns 2 and 4. Consider column 4 first,

$$\frac{4}{3} \Delta x^3 \tilde{a} - (-\tilde{a} \frac{4}{3} \Delta x^3) + \frac{\tilde{b}}{6} \Delta x^3 - (-\tilde{b} \frac{1}{6} \Delta x^3) = 0$$

$$\Rightarrow \frac{8}{3} \Delta x^3 \tilde{a} + \frac{1}{3} \tilde{b} \Delta x^3 = 0 \quad \text{or} \quad \frac{8}{3} \tilde{a} + \frac{1}{3} \tilde{b} = 0 \quad (\Delta x > 0)$$

$$\therefore 8\tilde{a} + \tilde{b} = 0 \rightarrow \textcircled{\text{I}}$$

We also want column (2) to sum upto 1, we have

$$2\Delta x \tilde{a} - (-2\Delta x \tilde{a}) + \tilde{b} \Delta x - (-\tilde{b} \Delta x) = 1$$

$$4\tilde{a} + 2\tilde{b} = \frac{1}{\Delta x} \rightarrow \textcircled{\text{II}}$$

$$\therefore \textcircled{\text{I}} - 2\textcircled{\text{II}} \Rightarrow \begin{aligned} 8\tilde{a} + \tilde{b} &= 0 \\ -8\tilde{a} + 4\tilde{b} &= 2/\Delta x \end{aligned}$$

$$-3\tilde{b} = -\frac{2}{\Delta x}$$

$$\Rightarrow \tilde{b} = \frac{2}{3\Delta x}$$

$$\therefore 8\tilde{a} - \tilde{b} = -\frac{2}{3\Delta x} \Rightarrow \boxed{\tilde{a} = -\frac{1}{12\Delta x}}$$

Using $\tilde{a} = -\frac{1}{12\Delta x}$ and $\tilde{b} = \frac{2}{3\Delta x}$ in the following manner

$$(**) \quad (a) \times \tilde{a} + (b) \times (-\tilde{a}) + (c) \times \tilde{b} + (d) \times (-\tilde{b})$$

will zero out columns 1, 3 and 5 since coefficients will be equal and opposite and will also zero out column 4 and sum up column 2's coefficients to 1 as per above calculations

$$\therefore \text{R.H.S} = f'(x)$$

Using these to evaluate the L.H.S., we have,

$$\text{L.H.S} = \tilde{a} \cdot f(x+2\Delta x) - \tilde{a} \cdot f(x-2\Delta x) + \tilde{b} \cdot f(x+\Delta x) - \tilde{b} \cdot f(x-\Delta x)$$

$$= -\frac{1}{12\Delta x} f(x+2\Delta x) - \left(-\frac{1}{12\Delta x} f(x-2\Delta x)\right) + \frac{2}{3\Delta x} f(x+\Delta x)$$

$$- \left(\frac{2}{3\Delta x} f(x-\Delta x)\right)$$

$$= \frac{1}{12\Delta x} \left(f(x-2\Delta x) - f(x+2\Delta x) \right)$$

$$+ \frac{2}{3\Delta x} \left(f(x+\Delta x) - f(x-\Delta x) \right)$$

$$= -\frac{1}{3} \left[\frac{f(x+2\Delta x) - f(x-2\Delta x)}{4\Delta x} \right]$$

$$+ \frac{4}{3} \left[\frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} \right]$$

which proves the expression given!

As far as the higher order terms, each of (a), (b), (c) and (d) have $\mathcal{O}(\Delta x^5)$

However, when we multiply by coefficients as in (**),

since each of the coefficients has $\frac{1}{\Delta x}$, the higher order terms become $\Theta(\Delta x^4)$.

This term is on the R.H.S, which becomes $-\Theta(\Delta x^4)$ on the L.H.S

But, this negative sign can be absorbed into the Big-O notation giving $\Theta(\Delta x^4)$ on the L.H.S

\therefore We get L.H.S = R.H.S \Rightarrow

$$f'(x) = \frac{4}{3} \left[\frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} \right] - \frac{1}{3} \left[\frac{f(x+2\Delta x) - f(x-2\Delta x)}{4\Delta x} \right] + \Theta(\Delta x^4)$$

<2.> 4th Order central difference (2nd derivative)
Consider the 4 Taylor's expansions,

$$(a) f(x+2\Delta x) = f(x) + 2\Delta x f'(x) + 2\Delta x^2 f''(x) + \frac{4}{3} \Delta x^3 f'''(x) + \frac{2}{3} \Delta x^4 f^{(4)}(x) + \frac{4}{15} \Delta x^5 f^{(5)}(x) + \Theta(\Delta x^6)$$

$$(b) f(x-2\Delta x) = f(x) - 2\Delta x f'(x) + 2\Delta x^2 f''(x) - \frac{4}{3} \Delta x^3 f'''(x) + \frac{2}{3} \Delta x^4 f^{(4)}(x) - \frac{4}{15} \Delta x^5 f^{(5)}(x) + \Theta(\Delta x^6)$$

$$(c) f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{1}{2} \Delta x^2 f''(x) + \frac{1}{6} \Delta x^3 f'''(x) + \frac{1}{24} \Delta x^4 f^{(4)}(x) + \frac{1}{120} \Delta x^5 f^{(5)}(x) + \Theta(\Delta x^6)$$

$$(d) f(x-\Delta x) = f(x) - \Delta x f'(x) + \frac{1}{2} \Delta x^2 f''(x) - \frac{1}{6} \Delta x^3 f'''(x) + \frac{1}{24} \Delta x^4 f^{(4)}(x) - \frac{1}{120} \Delta x^5 f^{(5)}(x) + \Theta(\Delta x^6)$$

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$$(c) f(x) = f(x)$$

We can zero out columns 2, 4 and 6 by multiplying with same coefficients of $(\tilde{a}, \tilde{a}, \tilde{b}, \tilde{b})$ as these columns have coefficients of equal magnitude but opposite sign

This leaves us with columns 1, 3 and 5 where all coefficients are positive.

For column 1, we would get $(2\tilde{a} + 2\tilde{b})f(x)$. To eliminate this we can use equation (e) and multiply by coefficient $-(2\tilde{a} + 2\tilde{b})$ to cancel out coefficients of equations (a) to (d).

So, finally for columns 3 and 5 we solve for \tilde{a} and \tilde{b} such that coefficients of 3 sum upto 1 and those of 5 sum upto 0.

$$\text{for col. 3, } 2\Delta x^2 \tilde{a} + 2\Delta x^2 \tilde{a} + \frac{1}{2}\Delta x^2 \tilde{b} + \frac{1}{2}\Delta x^2 \tilde{b} = 1$$

$$4\Delta x^2 \tilde{a} + \Delta x^2 \tilde{b} = 1$$

$$\text{or } 4\tilde{a} + \tilde{b} = \frac{1}{\Delta x^2} \rightarrow \textcircled{\text{I}}$$

$$\text{for col. 5, } \frac{2}{3}\Delta x^4 \tilde{a} + \frac{2}{3}\Delta x^4 \tilde{a} + \frac{1}{24}\Delta x^4 \tilde{b} + \frac{1}{24}\Delta x^4 \tilde{b} = 0 \dots (\Delta x^4 > 0)$$

$$\frac{4}{3}\tilde{a} + \frac{1}{12}\tilde{b} = 0$$

$$16\tilde{a} + \tilde{b} = 0 \rightarrow \textcircled{\text{II}}$$

$$4 \cdot \textcircled{\text{I}} - \textcircled{\text{II}} \Rightarrow 16\tilde{a} + 4\tilde{b} = 4/\Delta x^2$$

$$-16\tilde{a} + \tilde{b} = 0$$

$$\underline{\quad \quad \quad} \quad \underline{\quad \quad \quad} \quad \underline{\quad \quad \quad}$$

$$3\tilde{b} = \frac{4}{\Delta x^2} \Rightarrow \boxed{\tilde{b} = \frac{4}{3\Delta x^2}}$$

$$\therefore 16\tilde{a} - \tilde{b} = -\frac{4}{3\Delta x^2} \Rightarrow \tilde{a} = \frac{-\frac{4}{3 \cdot 16 \cdot \Delta x^2}}{\frac{4}{4}} = \boxed{-\frac{1}{12\Delta x^2}}$$

$$\therefore (a) \times \tilde{a} + (b) \times \tilde{a} + (c) \times \tilde{b} + (d) \times \tilde{b} + (e) \times (-2\tilde{a} - 2\tilde{b})$$

$$\text{will yield, R.H.S} = f''(x) + \frac{\Theta(\Delta x^6)}{\Delta x^2}$$

$$= f''(x) + \Theta(\Delta x^4)$$

$$\text{and L.H.S} = \tilde{a} [f(x+2\Delta x) + f(x-2\Delta x)] + \tilde{b} [f(x+\Delta x) + f(x-\Delta x)] - 2\tilde{a}f(x) - 2\tilde{b}f(x)$$

$$= -\frac{1}{12\Delta x^2} [f(x+2\Delta x) + f(x-2\Delta x)] + \frac{4}{3\Delta x^2} [f(x+\Delta x) + f(x-\Delta x)] - 2\left(-\frac{1}{12\Delta x^2}\right)f(x) - 2\left(\frac{4}{3\Delta x^2}\right)f(x)$$

$$= \frac{1}{12\Delta x^2} \left[-f(x+2\Delta x) - f(x-2\Delta x) + 16f(x+\Delta x) + 16f(x-\Delta x) - 2f(x) - 32f(x) \right]$$

$$= \frac{1}{12\Delta x^2} \left[-f(x+2\Delta x) + 16f(x+\Delta x) - 30f(x) + 16f(x-\Delta x) - f(x-2\Delta x) \right]$$

Taking the $\Theta(\Delta x^4)$ to LHS and absorbing the negative sign, the final expression is,

$$\boxed{f''(x) = \frac{-f(x+2\Delta x) + 16f(x+\Delta x) - 30f(x) + 16f(x-\Delta x) - f(x-2\Delta x)}{12\Delta x^2} + \Theta(\Delta x^4)}$$

Q3. 3rd order forward difference for 1st derivative

Consider the following Taylor's approximations,

$$e_1: f(x) = f(x)$$

$$e_2: f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{1}{2} \Delta x^2 f''(x) + \frac{1}{6} \Delta x^3 f'''(x) + \Theta(\Delta x^4)$$

$$e_3: f(x+2\Delta x) = f(x) + 2\Delta x f'(x) + 2\Delta x^2 f''(x) + \frac{4}{3} \Delta x^3 f'''(x) + \Theta(\Delta x^4)$$

$$e_4: f(x+3\Delta x) = f(x) + 3\Delta x f'(x) + \frac{9}{2} \Delta x^2 f''(x) + \frac{9}{2} \Delta x^3 f'''(x) + \Theta(\Delta x^4)$$

We want to make column 1, 3 and 4 sum to zero and column 2 sum to 1.

Consider 2, 3 and 4.

$$\text{for col. 2, } a \Delta x + b 2\Delta x + c 3\Delta x = 1$$

$$a + 2b + 3c = \frac{1}{\Delta x} \rightarrow \text{(I)}$$

$$\text{for col. 3, } \frac{a}{2} \Delta x^2 + 2b \Delta x^2 + \frac{9c}{2} \Delta x^2 = 0 \quad \dots (\Delta x^2 > 0)$$

$$a + 4b + 9c = 0 \rightarrow \text{(II)}$$

$$\text{for col. 4, } \frac{a}{6} \Delta x^3 + \frac{4b}{3} \Delta x^3 + \frac{9c}{2} \Delta x^3 = 0 \quad \dots (\Delta x^3 \neq 0)$$

$$a + 8b + 27c = 0 \rightarrow \text{(III)}$$

$$\text{(III)} - \text{(II)} \Rightarrow a + 8b + 27c = 0$$

$$= a + 4b + 9c = 0$$

$$4b + 18c = 0$$

$$2b + 9c = 0 \Rightarrow b = -\frac{9}{2}c$$

$$\begin{array}{rcl} \textcircled{\text{II}} - \textcircled{\text{I}} & \Rightarrow & a + 4b + 9c = 0 \\ & & -a + 2b + 3c = \frac{1}{\Delta x} \\ \hline & & 2b + 6c = -\frac{1}{\Delta x} \end{array}$$

substituting $b = -\frac{9}{2}c$,

$$2\left(-\frac{9}{2}c\right) + 6c = -\frac{1}{\Delta x}$$

$$-9c + 6c = -\frac{1}{\Delta x}$$

$$-3c = -\frac{1}{\Delta x} \Rightarrow \boxed{c = \frac{1}{3\Delta x}}$$

$$\therefore b = -\frac{9}{2}c = -\frac{9}{2} \cdot \frac{1}{3\Delta x} = \boxed{-\frac{3}{2\Delta x}}$$

$$\begin{aligned} \text{from } \textcircled{\text{II}}, \quad a &= -4b - 9c = -4\left(-\frac{3}{2\Delta x}\right) - 9\left(\frac{1}{3\Delta x}\right) \\ &= \frac{6}{\Delta x} - \frac{3}{\Delta x} = \boxed{\frac{3}{\Delta x}} \end{aligned}$$

Using the following,

$e_1 x - (a+b+c) + e_2 x a + e_3 x b + e_4 x c$
will zero out columns 1, 3 and 4 and sum up coefficients of column 2 to 1.

$$\therefore \text{R.H.S} = f'(x) + \frac{\Theta(\Delta x^4)}{\Delta x} = f'(x) + \Theta(\Delta x^3)$$

$$\begin{aligned} \text{and L.H.S} &= -(a+b+c)f(x) + a f(x+\Delta x) + b f(x+2\Delta x) \\ &\quad + c f(x+3\Delta x) \\ &= -\left(\frac{3}{\Delta x} - \frac{3}{2\Delta x} + \frac{1}{3\Delta x}\right)f(x) + \frac{3}{\Delta x} f(x+\Delta x) \\ &\quad - \frac{3}{2\Delta x} f(x+2\Delta x) + \frac{1}{3\Delta x} f(x+3\Delta x) \end{aligned}$$

$$\therefore \text{L.H.S} = - \left(\frac{18 - 9 + 2}{6\Delta x} \right) f(x) + \frac{18}{6\Delta x} f(x+\Delta x) \\ - \frac{9}{6\Delta x} f(x+2\Delta x) + \frac{2}{6\Delta x} f(x+3\Delta x)$$

$$= \frac{2f(x+3\Delta x) - 9f(x+2\Delta x) + 18f(x+\Delta x) - 11f(x)}{6\Delta x}$$

$$\therefore f'(x) = \frac{2f(x+3\Delta x) - 9f(x+2\Delta x) + 18f(x+\Delta x) - 11f(x)}{6\Delta x} + O(\Delta x^3)$$