Numerical Differentiation: Taylor expansion about $x_{j-1}$.

$$f(x) = f(x_{j-1}) + f'(x_{j-1})(x - x_{j-1}) + O(h^2)$$

@ $x = x_j$,

$$f(x_j) = f(x_{j-1}) + f'(x_{j-1})(x_j - x_{j-1}) + O(h^2)$$

$$f(x_j) - f(x_{j-1}) = f'(x_{j-1})\, h + O(h^2)$$

$$\boxed{\frac{1}{h} \cdot O(h^2) = O(h)}$$

Dividing by $h$,

$$\frac{f(x_j) - f(x_{j-1})}{h} = f'(x_{j-1}) + O(h)$$

$$f'(x_{j-1}) = \frac{f(x_j) - f(x_{j-1})}{h} + O(h)$$

Replacing $j$ with $j+1$,

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{h} + O(h)$$

So we shall take (ignoring $O(h)$)

$$\boxed{f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{h}}$$

This is called forward difference formula

Now again consider Taylor series expansion about $x_{j+1}$

$$f(x) = f(x_{j+1}) + f'(x_{j+1})\cdot(x - x_{j+1}) + O(h^2)$$

@ $x = x_j$

$$f(x_j) = f(x_{j+1}) + f'(x_{j+1})\,(\cancel{h}\, x_j - x_{j+1}) + O(h^2).$$

$$f(x_j) = f(x_{j+1}) + f'(x_{j+1})\,(-h) + O(h^2)$$

$$f(x_j) - f(x_{j+1}) = -h\, f'(x_{j+1}) + O(h^2)$$

Dividing by $-h$,

$$\frac{f(x_j) - f(x_{j+1})}{-h} = f'(x_{j+1}) + O(h)$$

$$\frac{f(x_{j+1}) - f(x_j)}{h} = f'(x_{j+1}) + O(h)$$

$$f'(x_{j+1}) = \frac{f(x_{j+1}) - f(x_j)}{h} + O(h)$$

Replacing $j$ with $j-1$

$$f'(x_j) = \frac{f(x_j) - f(x_{j-1})}{h} + O(h)$$

Ignoring $O(h)$ terms

$$\boxed{f'(x_j) = \frac{f(x_j) - f(x_{j-1})}{h}}$$

This is called backward difference formula

Now consider Taylor's Series expansion about $x_j$.

$$f(x) = f(x_j) + f'(x_j)(x - x_j) + \frac{1}{2} f''(x_j)(x - x_j)^2 + O(h^3)$$

@ $x = x_{j+1}$

$$f(x_{j+1}) = f(x_j) + f'(x_j)\underbrace{(x_{j+1} - x_j)}_{h} + \frac{1}{2} f''(x_j)\underbrace{(x_{j+1} - x_j)^2}_{h^2} + O(h^3) \longrightarrow (A)$$

@ $x = x_{j-1}$

$$f(x_{j-1}) = f(x_j) + f'(x_j)(x_{j-1} - x_j) + \frac{1}{2} f''(x_j)(x_{j-1} - x_j)^2 + O(h^3)$$

$$= f(x_j) - f'(x_j)\underbrace{(x_j - x_{j-1})}_{h} + \frac{1}{2} f''(x_j)\underbrace{(x_j - x_{j-1})^2}_{h^2} + O(h^3) \longrightarrow (B)$$

(A) − (B)

$$f(x_{j+1}) - f(x_{j-1}) = 2 f'(x_j)\, h + O(h^3)$$

$$\frac{f(x_{j+1}) - f(x_{j-1})}{2h} = f'(x_j) + O(h^2)$$

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_{j-1})}{2h}$$

This is called central difference formula.

- Forward and Backward difference are first order (you saw $O(h)$)
- Central difference is 2nd order (you saw $O(h^2)$)

Again consider Taylor series expansion about $x_{j+1}$

$$f(x) = f(x_j) + f'(x_j)(x-x_j) + \frac{1}{2} f''(x_j)(x-x_j)^2 + \frac{1}{6} f'''(x_j)(x-x_j)^3 + O(h^4)$$

at $x = x_{j+1}$

$$f(x_{j+1}) = f(x_j) + f'(x_j)(x_{j+1}-x_j) + \frac{1}{2} f''(x_j)(x_{j+1}-x_j)^2 + \frac{1}{6} f'''(x_j)(x_{j+1}-x_j)^3 + O(h^4) \quad \longrightarrow (A)$$

at $x = x_{j-1}$

$$f(x_{j-1}) = f(x_j) + f'(x_j)(x_{j-1}-x_j) + \frac{1}{2} f''(x_j)(x_{j-1}-x_j)^2 + \frac{1}{6} f'''(x_j)(x_{j-1}-x_j)^3 + O(h^4) \quad \longrightarrow (B)$$

(A) becomes

$$f(x_{j+1}) = f(x_j) + h f'(x_j) + \frac{h^2}{2} f''(x_j) + \frac{h^3}{6} f'''(x_j) + O(h^4)$$

(B) becomes

$$f(x_{j-1}) = f(x_j) - h f'(x_j) + \frac{h^2}{2} f''(x_j) - \frac{h^3}{6} f'''(x_j) + O(h^4)$$

Adding both:

$$f(x_{j+1}) + f(x_{j-1}) = 2 f(x_j) + h^2 f''(x_j) + O(h^4)$$

$$f(x_{j+1}) - 2 f(x_j) + f(x_{j-1}) = h^2 f''(x_j) + O(h^4)$$

Dividing by $h^2$,

$$\frac{f(x_{j+1}) - 2 f(x_j) + f(x_{j-1})}{h^2} = f''(x_j) + O(h^2)$$

Ignoring higher terms,

$$\boxed{f''(x_j) = \cancel{f}\ \frac{f(x_{j+1}) - 2 f(x_{j-1}) + f(x_{j-1})}{h^2}}$$

This is a formula for 2nd order derivative.

Ex: $f(x) = x^2$

Let $x_j = x$, $x_{j+1} = x+h$, $x_{j-1} = x-h$

$f(x_j) = f(x) = x^2$, $f(x_{j+1}) = (x+h)^2$, $f(x_{j-1}) = (x-h)^2$

1. First order derivative with forward difference formula

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{h}$$

$$= \frac{(x+h)^2 - x^2}{h} = \frac{2xh + h^2}{h} = 2x + h.$$

2. First order derivative with backward difference formula

$$f'(x_j) = \frac{f(x_j) - f(x_{j-1})}{h}$$

$$= \frac{x^2 - (x-h)^2}{h} = \frac{2xh - h^2}{h} = 2x - h$$

3. Central difference formula for 1st order derivative:

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_{j-1})}{2h}$$

$$= \frac{(x+h)^2 - (x-h)^2}{2h} = \frac{4xh}{2h} = 2x.$$

4. 2nd order derivative

$$f''(x_j) = \frac{f(x_{j+1}) - 2f(x_j) + f(x_{j-1})}{h^2}$$

$$= \frac{(x+h)^2 - 2x^2 + (x-h)^2}{h^2} = \frac{2h^2}{h^2} = 2$$