4. Discretization: step 2—derivation of FDAs

- Consider 4 FDAs:
  - 3 for first derivative
  - 1 for second derivative
- First write down and demonstrate level of accuracy, then illustrate one technique for derivation
- Formula here will be for x derivs, but will work for derivs in *any* coordinate direction (e.g. t)

4.1 FIRST ORDER FORWARD FDA for first derivative $f'(x)$

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

- "*forward* difference" since we use a value "forward" of x, i.e. $x + \Delta x$ to compute the approximation
- Grid function notation

$$f'_j \equiv f'(x_j) \approx \frac{f_{j+1} - f_j}{\Delta x}$$

- Use $\to$ to denote "is replaced with"—have first of three FDA formulae for $f'(x)$

$$\boxed{f'(x_j) \to \frac{f_{j+1} - f_j}{\Delta x}} \tag{1}$$

- Accuracy?
- Use Taylor series: $h \to \Delta x$ in eqn (TS)

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

- From (1) we have

$$\begin{aligned} \frac{f(x+\Delta x) - f(x)}{\Delta x} &= f'(x) + \frac{1}{2}\Delta x f''(x) + \frac{1}{6}\Delta x^2 f'''(x) + O(\Delta x^3) \\ &= f'(x) + \frac{1}{2}\Delta x f''(x) + O(\Delta x^2) \\ &= f'(x) + O(\Delta x) \end{aligned}$$

- Error term $O\Delta x$ means we have *first order* accurate approximation for the derivative of $f(x)$ at x
- I.e. as $\Delta x \to 0$ error in approximation will tend to decrease *linearly* in Δx, e.g. $\Delta x \to \Delta x/2$, error $\to$ error/2

4.2 FIRST ORDER BACKWARD FDA for first derivative, $f'(x)$

- Similar to previous approximation, but now we "backwards difference"

$$f'(x) \approx \frac{f(x) - f(x - \Delta x)}{\Delta x}$$

- Grid function notation

$$f_j' \equiv f'(x_j) \approx \frac{f_j - f_{j-1}}{\Delta x}$$

- Second FDA formula for $f'(x)$

$$\boxed{f'(x_j) \to \frac{f_j - f_{j-1}}{\Delta x}} \tag{2}$$

- Accuracy?
- Again, use Taylor series

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

- From (2) we have

$$\begin{aligned} \frac{f(x) - f(x - \Delta x)}{\Delta x} &= f'(x) - \frac{1}{2}\Delta x f''(x) + O(\Delta x^2) \\ &= f'(x) + O(\Delta x) \end{aligned}$$

- Also a *first order* accurate approximation for the derivative of $f(x)$ at x.

4.3 SECOND ORDER CENTRED FDA for first derivative, $f'(x)$

- Have two distinct first-order approximations for $f'(x)$
- Intuitively, if we take the average of formulae (1) and (2) we should get another approximation
- Try

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

- Grid function notation

$$f'_j \equiv f'(x_j) \approx \frac{f_{j+1}-f_{j-1}}{2\Delta x}$$

- Third FDA formula for $f'(x)$

$$\boxed{f'(x_j) \to \frac{f_{j+1}-f_{j-1}}{2\Delta x}} \qquad (3)$$

- Accuracy?
- Taylor series

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

- From (3) we have

$$\begin{aligned}\frac{f(x+\Delta x)-f(x-\Delta x)}{2\Delta x} &= f'(x)+\frac{1}{6}\Delta x^2 f'''(x)+O(\Delta x^4)\\ &= f'(x)+O(\Delta x^2)\end{aligned}$$

- So this is a *second order* approximation of the first derivative $f'(x)$ at x; i.e. as $\Delta x \to 0$ error in the approximation will tend to decrease *quadratically* in Δx, e.g. $\Delta x \to \Delta x/2$, error $\to$ error/4
- Approximation is called "centred": *structure* of formula is *symmetric* about point of approximation (i.e. we use both forward and backward values).