Numerical differentiation

We will show:

- First derivative : $\left.\frac{du}{dx}\right|_{x_i} = u'_i = \begin{cases} \frac{u_{i+1} - u_i}{h} + O(h) & \text{(F.E.)} \\ \frac{u_i - u_{i-1}}{h} + O(h) & \text{(B.E.)} \\ \frac{u_{i+1} - u_{i-1}}{2h} + O(h^2) & \text{(3 p.)} \end{cases}$

- Second derivative : $\left.\frac{d^2u}{dx^2}\right|_{x_i} = u''_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + O(h^2)$

- Definition of Taylor expansion of f around x

$$f(x+h) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(x)\, h^n$$

factorial

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

An aside on notation :

$f(x+h) = f(x) + f'(x)h + O(h^2)$ (exact)

$f(x+h) \approx f(x) + f'(x)h$ (approx. with truncation error $O(h^2)$)

- Can now find expression for $f'(x)$:

$$f(x+h) = f(x) + f'(x)\,h + \mathcal{O}(h^2)$$

$$\Rightarrow \quad f'(x) = \frac{f(x+h) - f(x) - \mathcal{O}(h^2)}{h}$$

$$\boxed{f_2'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)}$$

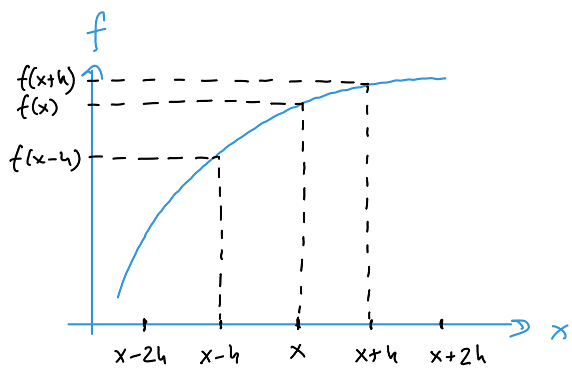
Note power of h!

- Compare to def.

$$f'(x) \equiv \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- Discretize
- $f \to u$ $\quad u_i' = \dfrac{u_{i+1} - u_i}{h} + \mathcal{O}(h)$

- This is the forward, two-point expression for the first derivative



- Could have used the points x and $x-h$

$$\Rightarrow \quad \boxed{f_2'(x) = \frac{f(x) - f(x-h)}{h} + \mathcal{O}(h)}$$

- Discr.
- $f \to u$

$$u_i' = \frac{u_i - u_{i-1}}{h} + \mathcal{O}(h)$$

- This is the backward, two-point expression

- Let's test it: $f(x) = a_0 + a_1 x$

Skip?

  - Exact: $f'(x) = a_1$

  - Approx, forward formula:

$$f_2'(x) \approx \frac{f(x+h) - f(x)}{h} = \frac{(\cancel{a_0} + \cancel{a_1 x} + a_1 h) - (\cancel{a_0} + \cancel{a_1 x})}{h}$$

$$= \frac{a_1 h}{h} = a_1$$

$$f_2'(x) \approx a_1$$

Exactly correct for a linear function (as you'd expect...)

- Let's test it again: $a_0 + a_1 x + a_2 x^2$

  - Exact: $f'(x) = a_1 + 2a_2 x$

  - Approx:

$$f_2(x) \approx \frac{f(x+h) - f(x)}{h}$$

$$= \frac{[\cancel{a_0} + a_1(\cancel{x}+h) + a_2(x+h)^2] - [\cancel{a_0} + \cancel{a_1 x} + a_2 x^2]}{h}$$

$$= \frac{a_1 \cancel{h} + \cancel{a_2 x^2} + 2a_2 x \cancel{h} + a_2 h^{\cancel{2}} - \cancel{a_2 x^2}}{\cancel{h}}$$

$$f_2(x) \approx a_1 + 2a_2 x + a_2 h$$

compare to exact result!

Skip ?

- We got an error of $O(h)$, as expected

- We can of course take h very small (small steps), but this can lead to roundoff errors in subtraction $f(x+h) - f(x)$ ... $\longrightarrow$ loss of precision

Illustration:

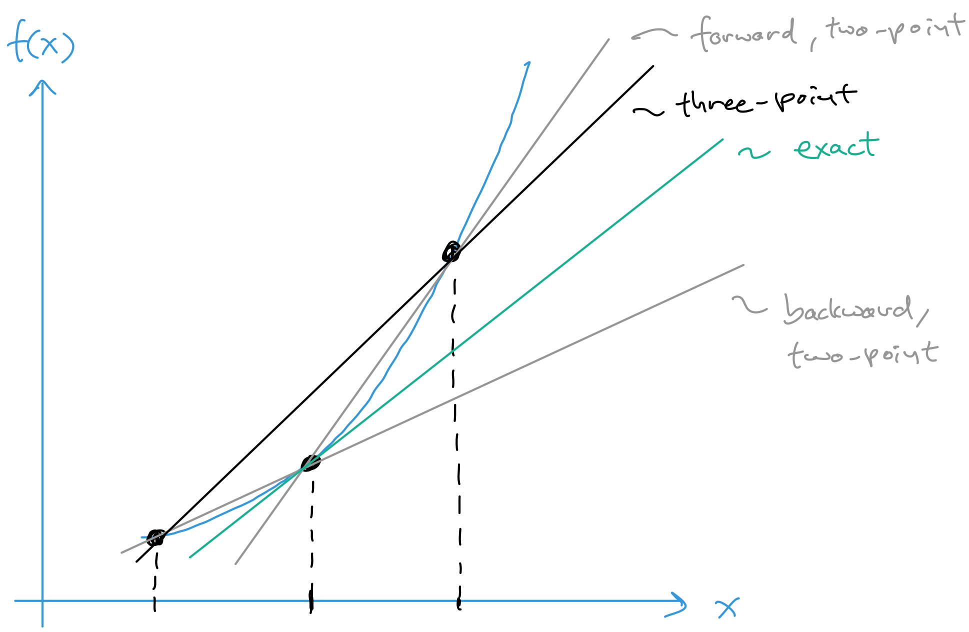
Say that for h quite small, we have

$$f(x) = 1.3000$$
$$f(x+h) = 1.3001$$

but you can only store numbers up to three decimals...

Then $f(x+h) - f(x) \rightarrow 1.300 - 1.300 = \underline{0}$

- But we can use more than two points...



- Three-point formula for $f'(x)$

- Start from Taylor exp. of both $f(x-h)$ and $f(x+h)$
  - $f(x-h) = f(x) - f'h + \frac{1}{2}f''h^2 - \frac{1}{6}f'''h^3 + O(h^4)$
  - $f(x+h) = f(x) + f'h + \frac{1}{2}f''h^2 + \frac{1}{6}f'''h^3 + O(h^4)$

- Subtract :

$$f(x+h) - f(x-h) = 2f'h + \frac{2}{6}f'''h^3 + O(h^5)$$

Note !

- Rearrange for f' :

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

$$\boxed{f_3'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)}$$

- Discr.
  - $f \to u$

$$u' = \frac{u_{i+1} - u_{i-1}}{2h} \quad O(h^2)$$

- Three-point formula for first derivative
  - Truncation error for f_3' is $O(h^2)$, compared to $O(h)$ for f_2'
  - Price to pay: Need to evaluate f at $f(x-h)$ in addition to $f(x+h)$
- Similarly, can obtain f_5' with truncation error $O(h^4)$, with the price of two more evaluations of f compared to f_3', etc.

[Strike balance between accuracy and time !]

- Second derivative

- Add $f(x+h) + f(x-h)$

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

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

$$f(x+h) + f(x-h) = 2f + f''h^2 + \mathcal{O}(h^4)$$

$$\Rightarrow \boxed{f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2)}$$

$$\frac{\mathcal{O}(h^4)}{h^2}$$

- Discr.
- $f \to u$

$$\boxed{u''_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \mathcal{O}(h^2)}$$