Numerical differentiation

Chapter 3.1 in Morten's notes

Main result:

- First derivative: $$\left.\frac{du}{dx}\right|_{x_i} = u_i' = \begin{cases} \dfrac{u_{i+1} - u_i}{h} + \mathcal{O}(h) & \text{(Two-point, forward diff.)} \\[2ex] \dfrac{u_i - u_{i-1}}{h} + \mathcal{O}(h) & \text{(Two-point, backward diff.)} \\[2ex] \dfrac{u_{i+1} - u_{i-1}}{2h} + \mathcal{O}(h^2) & \text{(Three-point)} \end{cases}$$

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

- Starting point: Taylor exp. of u around x

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

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

An aside on notation:

$$u(x+h) = u(x) + u'(x)h + \mathcal{O}(h^2) \quad \text{(exact)}$$

$$u(x+h) \approx u(x) + u'(x)h \quad \left(\text{approximation with truncation error } \mathcal{O}(h^2)\right)$$

- Can get expression for $u'(x)$:

$$u(x+h) = u(x) + u'(x)h + O(h^2)$$

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

$$\boxed{u'(x) = \frac{u(x+h) - u(x)}{h} + O(h)}$$

Note power of h

Compare to definition

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

- Discretize
  $u(x) \to u_i$

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

Two-point, forward difference

- We could have uses the points x and $x-h$

$$\Rightarrow \boxed{u'(x) = \frac{u(x) - u(x-h)}{h} + O(h)}$$

Discretize:

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

Two-point, backward difference

- Quick illustration of forward diff. method:

Example: $u(x) = a_0 + a_1 x + a_2 x^2$

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

- Approx: $u'(x) \approx \dfrac{u(x+h) - u(x)}{h}$

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

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

$$\underline{u'(x) \approx a_1 + 2a_2 x + \underset{\sim\sim}{a_2 h}}$$

- Compare to exact result: we got it wrong by an $O(h)$ term, as expected.

- This <u>truncation error</u> gets smaller when we take $h \to 0$, but this can lead to <u>roundoff errors</u> in the subtraction $u(x+h) - u(x)$ ... $\longrightarrow$ loss of precision

(We'll return to this.)

- Can use more than two points to comp. $u'(x)$:
  - Starting point: Taylor expansions
    - $u(x+h) = u(x) + u'h + \frac{1}{2}u''h^2 + \frac{1}{6}u'''h^3 + O(h^4)$
    - $u(x-h) = u(x) - u'h + \frac{1}{2}u''h^2 - \frac{1}{6}u'''h^3 + O(h^4)$
  - Subtract:

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

Note!

  - Rearrange:

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

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

$$\boxed{\text{Discretize: } u' = \frac{u_{i+1} - u_{i-1}}{2h} + O(h^2)}$$

Three-point formula for first derivative.

  - Truncation error is $O(h^2)$, compared to $O(h^2)$ for two-point methods
  - Price to pay: Need to evaluate u at both $u(x+h)$ and $u(x-h)$
  - Similarly, can get a <u>five-point formula</u> with error $O(h^4)$, etc.
  - Must strike balance between accuracy and time

- The second derivative

  - <u>Add</u> Taylor expansions for $u(x+h)$ and $u(x-h)$:

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

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

- Discretize

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