Overview

1. Numerical differentiation
    - First derivatives
    - Higher derivatives
2. Summary

Quiz this week! (Thu/Tue)

Recap

Functions vs numbers

Computers know nothing about the continuum

All our knowledge of a function $f(x)$ consists of

- a recipe for computing $y = f(x)$ for a given x
- rows of numbers x_i and their associated function values y_i

Numerical derivatives

Forward derivative $$\Delta_x^F f(x) = \frac{f(x+\delta) - f(x)}{\delta}$$

Backward derivative $$\Delta_x^B f(x) = \frac{f(x) - f(x-\delta)}{\delta}$$

Symmetric derivative $$\Delta_x^S f(x) = \frac{f(x+\delta) - f(x-\delta)}{2\delta}$$

Accuracy analysis

Theorem (Taylor's theorem)

For all positive integer n there exists a $\theta \in [0,1]$ such that

$$f(x+\delta) = f(x) + \delta f'(x) + \frac{\delta^2}{2} f''(x) + \ldots + \frac{\delta^n}{n!} f^{(n)}(x) + \frac{\delta^{n+1}}{(n+1)!} f^{(n+1)}(x+\theta\delta)$$

We do not know what θ is, but we do know that

$$\frac{1}{(n+1)!} f^{(n+1)}(x+\theta\delta) \quad \text{is some finite number}$$

We write

The error term

$$\frac{\delta^{n+1}}{(n+1)!} f^{(n+1)}(x+\theta\delta) = \mathcal{O}(\delta^{n+1})$$

Error on discrete derivatives

Use Taylor expansion:

$$
\begin{aligned}
f(x \pm \delta) &= f(x) \pm \delta f'(x) + \frac{\delta^2}{2} f''(x) + \mathcal{O}(\delta^3) \\
\Delta_x^F f(x) &= \frac{1}{\delta}\Big[f(x) + \delta f'(x) + \frac{\delta^2}{2} f''(x) + \mathcal{O}(\delta^3) - f(x) \Big] \\
&= f'(x) + \frac{\delta}{2} f''(x) + \mathcal{O}(\delta^2) = f'(x) + \mathcal{O}(\delta)
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\Delta_x^B f(x) &= \frac{1}{\delta}\Big[f(x) - \big(f(x) - \delta f'(x) + \frac{\delta^2}{2} f''(x) + \mathcal{O}(\delta^3) \big) \Big] \\
&= f'(x) - \frac{\delta}{2} f''(x) + \mathcal{O}(\delta^2) = f'(x) + \mathcal{O}(\delta) \\
\Delta_x^S f(x) &= \frac{1}{2\delta}\Big[f(x) + \delta f'(x) + \frac{\delta^2}{2} f''(x) - f(x) + \delta f'(x) - \frac{\delta^2}{2} f''(x) + \mathcal{O}(\delta^3) \Big] \\
&= f'(x) + \mathcal{O}(\delta^2)
\end{aligned}
$$

Error on discrete derivatives

Forward, backward and symmetric

$$\Delta_x^F f(x) = f'(x) + \mathcal{O}(\delta)$$
$$\Delta_x^B f(x) = f'(x) + \mathcal{O}(\delta)$$
$$\Delta_x^S f(x) = f'(x) + \mathcal{O}(\delta^2)$$

The forward and backward derivatives have errors of $\mathcal{O}(\delta)$,
while the symmetric derivative has errors of $\mathcal{O}(\delta^2)$.

Notation

We usually denote the accuracy by the order of the leading error term:

- Δ^F, Δ^B are accurate up to [errors of] $\mathcal{O}(\delta)$
- Δ^S is accurate up to $\mathcal{O}(\delta^2)$

Why use Δ^F, Δ^B?

Why would we ever want to use Δ^F, Δ^B?

- We have an irregular grid: $x_i - x_{i-1} \neq x_{i+1} - x_i$
- $f(x)$ is very expensive to evaluate; we have already evaluated it at x
- We cannot evaluate $f(x - \delta)$ (out of physical range)
- The symmetric derivative gives rise to unphysical artefacts, eg. spurious symmetries

Rounding errors

The discrete derivative is defined as a (small) difference between two (possibly large) numbers, divided by a small number

Alarm bells

- if δ is small, it will suffer from rounding errors
- so too will $x, x + \delta$
- $f(x + \delta) - f(x)$ will have rounding errors (usually $>$ machine precision)

Main lessons

- You can never compute a derivative to machine precision!
- Do not try to push your δ too small!

We will usually be working on fixed grids where $\delta \gg \varepsilon_m$
Our main worry is truncation errors $=$ accuracy

Second derivatives

$$\frac{d^2 f}{dx^2} = \frac{d}{dx}\left(\frac{df}{dx}\right) \quad \rightarrow \quad \Delta_x^{BFS}\left(\Delta_x^{BFS} f\right)$$

This gives 6 possible combinations (since $\Delta^a \Delta^b f = \Delta^b \Delta^a f$).
Only one is used:

$$\begin{aligned}
\Delta^2 f(x) \equiv \Delta^B \Delta^F f(x) &= \frac{\Delta^F f(x) - \Delta^F f(x-\delta)}{\delta} \\
&= \frac{f(x+\delta) - f(x) - \big(f(x) - f(x-\delta)\big)}{\delta^2}
\end{aligned}$$

The symmetric second derivative

$$\Delta^2 f(x) = \frac{f(x+\delta) - 2f(x) + f(x-\delta)}{\delta^2}$$

Accuracy analysis

We expand the Taylor series as before:

$$f(x \pm \delta) = f(x) \pm \delta f'(x) + \frac{\delta^2}{2} f''(x) \pm \frac{\delta^3}{6} f'''(x) + \frac{\delta^4}{24} f^{(4)}(x) + \mathcal{O}(\delta^5)$$

$$f(x+\delta) + f(x-\delta) - 2f(x) = \delta^2 f''(x) + \frac{\delta^4}{12} f^{(4)}(x) + \mathcal{O}(\delta^5)$$

Accuracy of second derivative

$$\Delta^2 f(x) = f''(x) + \frac{\delta^2}{12} f^{(4)}(x) + \mathcal{O}(\delta^3) = f''(x) + \mathcal{O}(\delta^2)$$

— accurate up to $\mathcal{O}(\delta^2)$!

Why none of the other 5?

- they are either asymmetric → $\mathcal{O}(\delta)$ errors
- or involve 2-hop terms → bigger absolute errors

Higher order formulae

- Higher order derivatives: not very common in physics
  - but can be constructed in same way
  - Korteweg–de Vries: $\partial_t \phi + \partial_x^3 \phi + 6\phi \partial_x \phi = 0$
- Higher order accuracy: not required very often
  - can be constructed using Taylor expansion to appropriate order, matching coeffs at each order
  - for example:

$$\frac{-f(x+2\delta) + 8f(x+\delta) - 8f(x-\delta) + f(x-2\delta)}{12\delta} = f'(x) + \mathcal{O}(\delta^4)$$

  - relevant in cases where reducing δ is impossible or very expensive, and function is very well-behaved
- Non-linearities are usually more important in practice
  - Euler equation: $\partial_t \vec{v} + (\vec{v} \cdot \nabla)\vec{v} + \frac{1}{\rho}\nabla p = 0$
  - Quantum Electrodynamics: $\nabla \quad \rightarrow \quad \nabla + ie\vec{A}$

Summary

- Forward derivative: $\Delta^F f(x) = [f(x+\delta) - f(x)]/\delta = f'(x) + \mathcal{O}(\delta)$
- Backward derivative: $\Delta^B f(x) = [f(x) - f(x-\delta)]/\delta = f'(x) + \mathcal{O}(\delta)$
- Symmetric derivative:
  $\Delta^S f(x) = [f(x+\delta) - f(x-\delta)]/(2\delta) = f'(x) + \mathcal{O}(\delta^2)$
- Accuracy analysis performed by Taylor series expansion
- Symmetric second derivative:
- Higher order expressions not very much used