Topic and contents

UNSW, School of Mathematics and Statistics

MATH2089 – Numerical Methods

Week 01 – Taylor polynomials / Finite differences

1. Order notations
   - As quantities get large
   - As quantities get small
2. Taylor polynomials
3. Finite difference approximations
   - Forward difference approximations to $f'(x)$
   - Central difference approximations to $f'(x)$
   - Truncation error vs. rounding error
   - Central difference approximation to $f''(x)$

- MATLAB M-files
  - `taylor1.m`
  - `taylor2.m`
  - `fdiff.m`

Some motivations

- In weather forecasting models, one needs to compute derivatives of a function approximately when you can evaluate the function values only.
- Methods: finite differences
- People needs to know how good the approximations are.
- To analyze the errors, we need to introduce the order notations, Taylor polynomial approximations, etc.

Order notation – limit $\to \infty$

Definition (Order notation)

- Big O: same order of magnitude

$$\alpha(n) = O(n^k) \iff \lim_{n\to\infty} \frac{|\alpha(n)|}{n^k} = K, \quad 0 < K < \infty$$

- Little o: smaller order of magnitude

$$\alpha(n) = o(n^k) \iff \lim_{n\to\infty} \frac{|\alpha(n)|}{n^k} = 0$$

Example (As $n \to \infty$)

- $\alpha = 3.2n^3 - 46.4n^2 + 376.9n, \quad \alpha = O(n^3)$
- $\alpha = -46.4n^2 + 376.9n + 20\pi, \quad \alpha = o(n^3), \quad \alpha = O(n^2)$
- $\alpha = 3.6n^{2.6}, \quad \alpha = o(n^3)$

Order notation – limit $\to 0$

Definition (Order notation)

- Big O: same order of magnitude:

$$\alpha(h) = O(h^k) \iff \lim_{h\to 0} \frac{|\alpha(h)|}{h^k} = K, \quad 0 < K < \infty$$

- Little o: smaller order of magnitude

$$\alpha(h) = o(h^k) \iff \lim_{h\to 0} \frac{|\alpha(h)|}{h^k} = 0$$

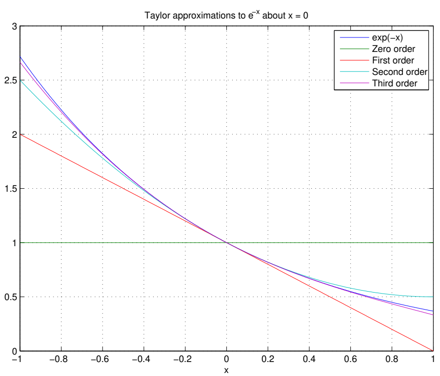
Example (As $h \to 0$)

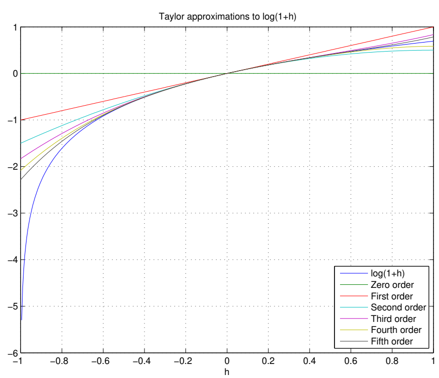
- $\alpha = 3.2h^3 - 46.4h^2 + 376.9h, \quad \alpha = O(h)$
- $\alpha = 3.2h^3 - 46.4h^2, \quad \alpha = o(h),\ \alpha = O(h^2)$
- $\alpha = 3.6h^{2.6}, \quad \alpha = o(h^2)$

Taylor approximations

Example (Taylor polynomial approximations)

- $\exp(-x) = 1 - x + \frac{x^2}{2} - \frac{x^3}{6} + O(x^4)$ `taylor1.m`
- $\log(1+h) = h - \frac{h^2}{2} + \frac{h^3}{3} - \frac{h^4}{4} + \frac{h^5}{5} + O(h^6)$ `taylor2.m`





- In general, we have (not necessarily convergent)

$$f(x) \approx f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2!}(x-x_0)^2 + \frac{f'''(x_0)}{3!}(x-x_0)^3 + \cdots$$

- Set $h = x - x_0$ and replace x by $x_0 + h$:

$$f(x_0+h) \approx f(x_0) + f'(x_0)h + \frac{f''(x_0)}{2!}h^2 + \frac{f'''(x_0)}{3!}h^3 + \cdots$$

Taylor approximation

Definition (Taylor approximation)

Let $f \in C^{n+1}([a,b])$ (all derivatives up to $n+1$ continuous on $[a,b]$). Then

$$\begin{aligned} f(x+h) &= \sum_{k=0}^{n} h^k \frac{f^{(k)}(x)}{k!} + h^{n+1}\frac{f^{(n+1)}(\zeta)}{(n+1)!} \quad \text{for some unknown } \zeta \in (a,b) \\ &= f(x) + hf'(x) + h^2\frac{f''(x)}{2!} + \cdots + h^n \frac{f^{(n)}(x)}{n!} + O\left(h^{n+1}\right) \\ &= \text{Taylor polynomial of degree } n + \text{remainder term} \end{aligned}$$

Forward difference approximations $f'(x)$

- Assume you can evaluate function values f
- Want to approximate $f'(x)$
- Assume $f \in C^2([a,b])$ and $x \in (a,b)$
- Taylor series

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\zeta), \qquad \zeta \in (a,b)$$

- Rearrange to get forward difference approximation of order $O(h)$

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(\zeta)$$

  - Stepsize $h > 0$
  - Truncation error $O(h)$

Central difference approximations $f'(x)$

- Assume $f \in C^3([a,b])$ and $x \in (a,b)$
- Taylor series

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

- Subtract
$$f(x+h) - f(x-h) = 2hf'(x) + O(h^3)$$
- Rearrange to get central difference approximation of order h^2

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

  - Truncation error $O(h^3)/(2h) = O(h^2)$

Example of difference approximations to $f'(x)$

Example (Difference approximations to $f'(x)$ for $f(x) = \log(1+x)$ at $x = 2$)

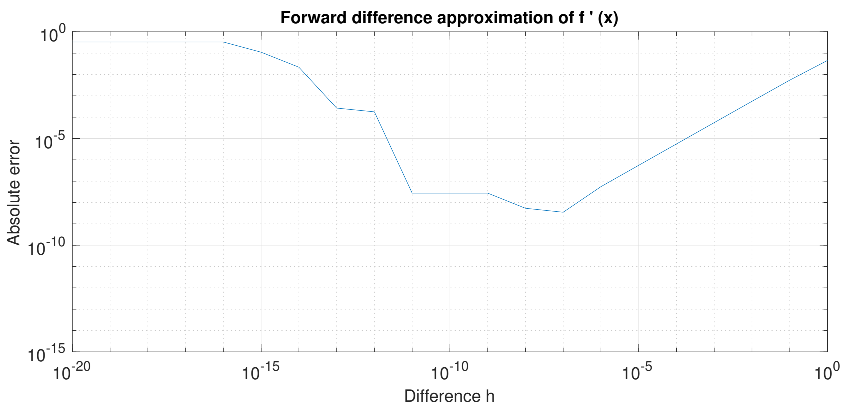
- MATLAB M-file `fdiff.m`: `linspace`, `plot`, anonymous function
- The plot shows the absolute errors

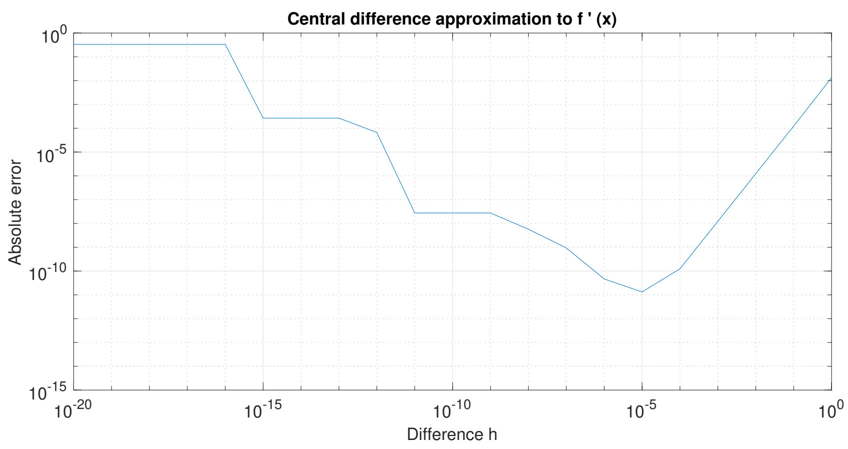
$$\left| \frac{f(2+h) - f(2)}{h} - f'(2) \right|$$

and

$$\left| \frac{f(2+h) - f(2-h)}{2h} - f'(2) \right|$$

Question What do you expect from the errors when $h \to 0$?





Forward difference error

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

- Rounding error $= RE(h) = O\left(\frac{\epsilon}{h}\right)$.
- Truncation error $= TE(h) = O(h)$.
- Total error $= O\left(\frac{\epsilon}{h}\right) + O(h)$.

Central difference error

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

- Rounding error $= RE(h) = O\left(\frac{\epsilon}{h}\right)$.
- Truncation error $= TE(h) = O(h^2)$.
- Total error $= O\left(\frac{\epsilon}{h}\right) + O(h^2)$.

Truncation vs. Rounding Error

- Truncation error $TE(h)$ from mathematical approximation
  - Forward difference $O(h)$
  - Central difference $O(h^2)$
  - Truncation error $\to 0$ as $h \to 0$
- Storing numbers on a computer has rounding error
  - rounding error in storing y is $\epsilon|y|$
- For h sufficiently small $x+h$ and x stored as the same number
  - $\implies f(x+h) - f(x) = 0$
  - $\implies$ error $= |f'(x)|$ ($= 1/3$ in Example)
- Rounding error $RE(h)$ from computer arithmetic
  - First derivative, forward difference $RE(h) = O(\epsilon/h)$
  - First derivative, central difference $RE(h) = O(\epsilon/h)$
  - Rounding error $\to \infty$ as $h \to 0$
- Total Error $E(h) = TE(h) + RE(h)$

Optimal stepsize – forward difference

- Choose finite difference stepsize to minimize total error $E(h)$
- Forward difference approximation to $f'(x)$
  - Minimize (where $c_1, c_2 > 0$ positive constants)

$$E(h) = O(h) + O(\epsilon/h) = c_1 h + \frac{c_2\epsilon}{h}$$

  - Stationary point

$$E'(h) = c_1 - \frac{c_2\epsilon}{h^2} = 0 \implies h = \left(\frac{c_2\epsilon}{c_1}\right)^{\frac{1}{2}} = O\left(\epsilon^{\frac{1}{2}}\right)$$

  - Minimum as

$$E''(h) = \frac{2c_2}{h^3} > 0$$

  - Optimal stepsize is $h^* = O\left(\epsilon^{\frac{1}{2}}\right) \implies E(h^*) = O\left(\epsilon^{\frac{1}{2}}\right)$
  - Double precision $\epsilon \approx 2 \times 10^{-16} \implies h^* \approx 1 \times 10^{-8}$

Optimal stepsize - central difference

- Central difference approximation to $f'(x)$

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

  - Truncation error $O(h^2)$, Rounding error $O(\epsilon/h)$
  - Minimize (where c_1, c_2 positive constants)

$$E(h) = O(h^2) + O(\epsilon/h) = c_1 h^2 + \frac{c_2\epsilon}{h}$$

  - Stationary point

$$E'(h) = 2c_1 h - \frac{c_2\epsilon}{h^2} = 0 \implies h = \left(\frac{c_2\epsilon}{c_1}\right)^{\frac{1}{3}} = O\left(\epsilon^{\frac{1}{3}}\right)$$

  - Minimum as

$$E''(h) = 2c_1 + \frac{2c_2}{h^3} > 0$$

  - Optimal stepsize is $h^* = O\left(\epsilon^{\frac{1}{3}}\right) \implies E(h^*) = O\left(\epsilon^{\frac{2}{3}}\right)$
  - Double precision $\epsilon \approx 2 \times 10^{-16} \implies h^* \approx 6 \times 10^{-6}$

Central difference approximation to $f''(x)$

- Assume $f \in C^4([a,b])$ and $x \in (a,b)$
- Taylor series

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{3!}f'''(x) + O(h^4) \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{3!}f'''(x) + O(h^4) \end{aligned}$$

- Add

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + O(h^4)$$

- Rearrange to get central difference approximation of order h^2

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

  - Truncation error $O(h^4)/(h^2) = O(h^2)$, Rounding error $O(\epsilon/h^2)$
  - Exercise: Optimal stepsize $h^* = O\left(\epsilon^{\frac{1}{4}}\right)$