Numerical Differentiation

MTHBD/CMPBD 423

- Derivation of the central difference formula for $f'(x_i)$ of order $h^2$. (Two function evaluations)

Assume $f \in C^3[a,b]$ and $x-h, x, x+h \in [a,b]$. Expanding $f(x+h)$ and $f(x-h)$ about $x$:

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f^{(3)}(\xi_1)h^3}{3!} \quad \text{where } \xi_1 \in [x, x+h] \quad (1)$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)h^2}{2!} - \frac{f^{(3)}(\xi_2)h^3}{3!} \quad \text{where } \xi_2 \in [x-h, x] \quad (2)$$

Subtracting (2) from (1) yields

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{f^{(3)}(\xi_1) + f^{(3)}(\xi_2)}{3!} h^3.$$

Since $f^{(3)}$ is continuous, the intermediate value theorem implies

$$\frac{f^{(3)}(\xi_1) + f^{(3)}(\xi_2)}{2} = f^{(3)}(\xi) \quad \text{where } \xi \in [x-h, x+h].$$

Now solving for $f'(x)$ yields

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f^{(3)}(\xi)}{3!} h^2$$

$$f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{f^{(3)}(\xi)}{3!} h^2$$

$$f'(x_i) = \frac{f_{i+1} - f_{i-1} + E_{\text{trunc}}(f, h)}{2h} + O(h^2)$$

as desired. The term $E_{\text{trunc}}(f, h)$ is called the Truncation Error. Above, the truncation error is order $h^2$.

- Derivation of the central difference formula for $f''(x_i)$ of order $h^2$. (Three function evaluations)

Adding (2) and (1) (where one more term is retained) yields

$$f(x+h) + f(x-h) = 2f(x) + f''(x)h^2 + \frac{f^{(4)}(\xi_1) + f^{(4)}(\xi_2)}{4!} h^4$$

$$= 2f(x) + f''(x)h^2 + \frac{2f^{(4)}(\xi)h^4}{4!} \quad \text{where } \xi \in [x-h, x+h].$$

Now solving for $f''(x)$ yields

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{f^{(4)}(\xi)}{12} h^2$$

$$f''(x_i) = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + O(h^2)$$
Derivation of the central difference formula for $f'(x_i)$ of order $h^4$. (Four function evaluations)

Expanding $f(x + h), f(x - h), f(x + 2h),$ and $f(x - 2h)$ in Taylor Series’ about $x$ and subtracting the results yields

$$f(x + h) - f(x - h) = 2f'(x)h + \frac{2f^{(3)}(x)h^3}{3!} + \frac{2f^{(5)}(\xi_1)h^5}{5!} \quad \text{where} \quad \xi_1 \in [x - h, x + h] \quad (3)$$

$$f(x + 2h) - f(x - 2h) = 4f'(x)h + \frac{16f^{(3)}(x)h^3}{3!} + \frac{64f^{(5)}(\xi_2)h^5}{5!}. \quad \text{where} \quad \xi_2 \in [x - 2h, x + 2h] \quad (4)$$

Multiplying equation (3) by 8 and subtracting equation (4) yields

$$-f(x + 2h) + 8f(x + h) - 8f(x - h) + f(x - 2h) = 12f'(x)h + \frac{\left(16f^{(5)}(\xi_1) - 64f^{(5)}(\xi_2)\right)h^5}{120} \quad (5)$$

or

$$f'(x) = \frac{-f(x + 2h) + 8f(x + h) - 8f(x - h) + f(x - 2h)}{12h} + \frac{\left(64f^{(5)}(\xi_2) - 16f^{(5)}(\xi_1)\right)h^4}{12 \cdot 120} \quad (6)$$

$$f'(x_i) = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} + \frac{\left(64f^{(5)}(\xi_2) - 16f^{(5)}(\xi_1)\right)h^4}{12 \cdot 120} + O(h^4).$$

Note:

$$64f^{(5)}(\xi_2) - 16f^{(5)}(\xi_1) = 16 \left(4f^{(5)}(\xi_2) - f^{(5)}(\xi_1)\right)$$

$$= 48 \left(\frac{4}{3}f^{(5)}(\xi_2) - \frac{1}{3}f^{(5)}(\xi_1)\right)$$

Since $f^{(5)}$ is continuous, if $h$ is chosen small enough, $\varepsilon$ will be such that

$$\left(\frac{4}{3}f^{(5)}(\xi_2) - \frac{1}{3}f^{(5)}(\xi_1)\right) = \left(\frac{4}{3}(f^{(5)}(\xi_1) + \varepsilon) - \frac{1}{3}f^{(5)}(\xi_1)\right)$$

$$= f^{(5)}(\xi_1) + \frac{4\varepsilon}{3}$$

$$= f^{(5)}(\xi)$$

and the difference formula (with truncation error) can be written:

$$f'(x_i) = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} + \frac{f^{(5)}(\xi)h^4}{30} \quad \text{where} \quad \xi \in [x_{i-2}, x_{i+2}] \quad (7)$$
Determining an Optimal Step Size: $h_{opt}$

- **Numerical Method** for an Arbitrary Differencing Scheme.
  Define a decreasing sequence of step sizes $\{h_k\}_{k=1}^n$ such that $h_k \to 0$, and let

  $$D_k = \text{approximation to the derivative.}$$

  $D_k$ should be computed until

  $$|D_{N+1} - D_N| \geq |D_N - D_{N-1}|.$$  

  Then

  $$h_N \approx \text{the optimum step size } = h_{opt}.$$  

- **Analytic Method** for a Specific Differencing Scheme.
  Example: central differencing for $f'(x_i)$, $O(h^2)$.

  $$f'(x_i) \approx \frac{f_{i+1} - f_{i-1}}{2h}$$

  $$f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2h} + E(f, h)$$

  where $E(f, h)$ is the total error:

  $$E(f, h) = E_{\text{round}}(f, h) + E_{\text{trunc}}(f, h)$$

  $$= \frac{e_{i+1} - e_{i-1}}{2h} - \frac{h^2 f^{(3)}(\xi)}{6}$$

  Let $\varepsilon$ be a maximum of the rounding and/or measurement error. Then

  $$|e_{i-1}| \leq \varepsilon \quad \text{and} \quad |e_{i+1}| \leq \varepsilon.$$  

  Let $M$ be the max of the 3rd derivative of $f$ on $[a,b]$:

  $$M = \max_{a \leq x \leq b} \{|f^{(3)}(x)|\}.$$  

  Now we can say

  $$|E(f, h)| \leq \frac{\varepsilon}{h} + \frac{Mh^2}{6} = g(h).$$  

  The goal is then to minimize $g(h)$ by differentiating it and setting the result equal to zero.

  $$g'(h) = -\frac{\varepsilon}{h^2} + \frac{Mh}{3} = 0$$

  yields

  $$h_{opt} = \left(\frac{3\varepsilon}{M}\right)^{1/3}.$$
Example: Approximate the optimal step size for estimating the derivative of \( f(x) = e^x \) over the interval \([0,2]\) using second order (\(O(h^2)\)) central differencing and assume machine round-off error to have a maximum of \(10^{-15}\) (appropriate for MATLAB where machine zero is \(10^{-16}\)). Check this numerically with a graph of \( \log(h) \) -vs- \( \log(\text{error}) \) at \( x_i = 1 \).

\[
f'(x_i) = \frac{y_{i+1} - y_{i-1}}{2h} + E(f,h)
\]

\[
|e_{i-1}| \leq \varepsilon = 10^{-15}
\]

\[
|e_{i+1}| \leq \varepsilon = 10^{-15}
\]

\[
M = \max_{0 \leq x \leq 2} \{|f^{(3)}(x)|\} = \max_{0 \leq x \leq 2} \{|e^x|\} = e^2
\]

\[
h_{opt} = \left(\frac{3\varepsilon}{M}\right)^{1/3} \approx 10^{-5.13}
\]

Notes:

- The slope of \( \log(h) \) -vs- \( \log(\text{error}) \) at \( x_i = 1 \) is 2 as should be the case with an order \( h^2 \) method.
- This slope is only valid until round-off error starts effecting the results. Ie: For \( h < h_{opt} \).
- If there was no round-off error, the slope would be 2 for the entire domain of \( h \) values.
- You can’t do much better than \(10^{-10}\) error with our resources and an order \( h^2 \) method.
- If you want better accuracy, you should use a higher order differencing scheme.
- Numerical method of determining \( h_{opt} \) suggests \(10^{-5.5}\) is the optimal value.