CHAPTER SIX

Numerical Differentiation

Objectives

- Approximating higher derivatives
- Central-difference formula for $f''(x)$ of order $O(h^2)$
- Optimum step-size for central-difference formula for $f''(x)$ of order $O(h^2)$

Approximating higher derivatives

- Such as approximating $f''(x)$, $f'''(x)$, $f^{(4)}(x)$
- Follow same procedure done on approximating $f'(x)$
- Use Taylor expansions for $f(x+h), f(x-h), f(x+2h), f(x-2h) \dots\dots\dots etc$

Central-difference formula for $f''(x)$ of order $O(h^2)$

- Start with third degree Taylor expressions about x
- $f(x+h) = f(x) + f'(x)h + \frac{f''(x)h^2}{2!} + \frac{f'''(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \cdots$
- $f(x-h) = f(x) - f'(x)h + \frac{f''(x)h^2}{2!} - \frac{f'''(x)h^3}{3!} + \frac{f^{(4)}(x)h^4}{4!} + \cdots$
- $f(x+h) + f(x-h) = 2f(x) + 2\frac{f''(x)h^2}{2!} + 2\frac{f^{(4)}(x)h^4}{4!}$
- $f(x+h) + f(x-h) = 2f(x) + f''(x)h^2 + O(h^4)$

Central-difference formula for $f''(x)$ of order $O(h^2)$ - Cont'd

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

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

Central-difference formula for $f''(x)$ of order $O(h^2)$

- $\boxed{f''(x) = \frac{f_1 - 2f_0 + f_{-1}}{h^2}}$

$$f_k = f(x+kh)$$
$$f_1 = f(x+h)$$
$$f_0 = f(x)$$
$$f_{-1} = f(x-h)$$

Central-difference formula for $f''(x)$ of order $O(h^2)$ - Example

- Let $f(x) = \cos(x)$. Use central-difference formula for $f''(x)$ of order $O(h^2)$ with step size $h = 0.1,\ 0.01,$ and 0.001 to approximate $f''(0.8)$
- Note that the exact value of $f''(0.8) = -\cos(0.8) = -0.6967067093471$

- If $h = 0.01$ →
- $f''(0.8) = \frac{f(0.81) - 2f(0.8) + f(0.79)}{0.01^2}$

$$= -0.696690000$$

Table 6.5 Numerical Approximations to $f''(x)$ for Example 6.4

Step size	Approximation by formula (6)	Error using formula (6)
$h = 0.1$	-0.696126300	-0.000580409
$h = 0.01$	-0.696690000	-0.000016709
$h = 0.001$	-0.696000000	-0.000706709

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Table 6.3 Central-difference Formulas of Order $O(h^2)$

$$f'(x_0) \approx \frac{f_1 - f_{-1}}{2h}$$

$$f''(x_0) \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2}$$

$$f^{(3)}(x_0) \approx \frac{f_2 - f_1 + 2f_{-1} - f_{-2}}{2h^3}$$

$$f^{(4)}(x_0) \approx \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4}$$

Table 6.4 Central-difference Formulas of Order $O(h^4)$

$$f'(x_0) \approx \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h}$$

$$f''(x_0) \approx \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2}$$

$$f^{(3)}(x_0) \approx \frac{-f_3 + 8f_2 - 13f_1 + 13f_{-1} - 8f_{-2} + f_{-3}}{8h^3}$$

$$f^{(4)}(x_0) \approx \frac{-f_3 + 12f_2 - 39f_1 + 56f_0 - 39f_{-1} + 12f_{-2} - f_{-3}}{6h^4}$$

Optimum Step Size

- $f(x_0 + kh) = y_k + e_k$

- $f''(x) = \frac{y_1 - 2y_0 + y_{-1}}{h^2} + E(f, h)$

- $E(f, h) = \frac{e_1 - 2e_0 + e_{-1}}{h^2} + \frac{f^{(4)}(c)h^2}{12}$

- $|E(f, h)| \le \boxed{\frac{4\epsilon}{h^2} + \frac{Mh^2}{12}}$ $g(h)$

- For optimal value of h: $g'(h) = 0$ ➔ $\boxed{h = \left(\frac{48\epsilon}{M}\right)^{\frac{1}{4}}}$

Optimum Step Size - Example

- Let $f(x) = \cos(x)$, and $\epsilon = 0.5 \times 10^{-9}$. Find optimum step size for central-difference formula for $f''(x)$ of order $O(h^2)$.

- $\left|f^{(4)}(x)\right| \leq |\cos(x)| \leq 1 \quad \rightarrow M = 1$

- $h = (\frac{48\epsilon}{M})^{\frac{1}{4}} = (\frac{48 \times 0.5 \times 10^{-9}}{1})^{\frac{1}{4}} = 0.01244666$
- Note that from previous example, optimum step size $h = \ 0.01$

References

- [1] Mathews J. H. and Fink K. D. (1999). Numerical Methods using MATLAB, NJ: Prentice Hall

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