Lecture 15: Numerical Differentiation and Integration (Contd..)

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Approximation of Derivatives via Taylor's Theorem

By Taylor's Theorem, we have

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi), \tag{1}$$

where $\xi \in (x, x+h)$ and $f'' \in C^2((x, x+h))$. Rewrting (1) as

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

The formula

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}, \quad \text{(forward difference formula)} \tag{2}$$

provides an approximation to $f'(x)$. The term $-\frac{h}{2} f''(\xi)$ is called the truncation error (**T.E.**). Note that **T.E.** $= O(h)$.

Similarly, Taylor's Theorem gives

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

where $\xi \in (x-h, x)$ and $f'' \in C^2((x-h, x))$. Rewrting (3) as

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

The formula

$$T_E = \frac{h}{2} f''(\xi) = O(h)$$

$$f'(x) \approx \frac{f(x) - f(x-h)}{h}, \tag{4}$$

(backward difference formula)

provides an approximation to $f'(x)$. The term $\frac{h}{2} f''(\xi)$ is called the truncation error.

A better approximation to first derivative is obtained as follows:

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(\xi_1) && (5) \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(\xi_2), && (6) \end{aligned}$$

where $\xi_1 \in (x, x+h)$ and $\xi_2 \in (x-h, x)$. Subtracting (6) from (5), we have

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \underbrace{\frac{h^2}{12}[f'''(\xi_1) + f'''(\xi_2)]}. \tag{7}$$

$$\frac{h^2}{6}\left[\frac{f'''(\xi_1)+f'''(\xi_2)}{2}\right]$$

Assuming $f''' \in C([x-h, x+h])$, there exists some point $\xi \in [x-h, x+h]$ such that

$$f'''(\xi) = \frac{1}{2}[f'''(\xi_1) + f'''(\xi_2)].$$

$$= \frac{h^2}{6} f'''(\xi)$$

The expression (7) becomes

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(\xi).$$

Thus, the formula

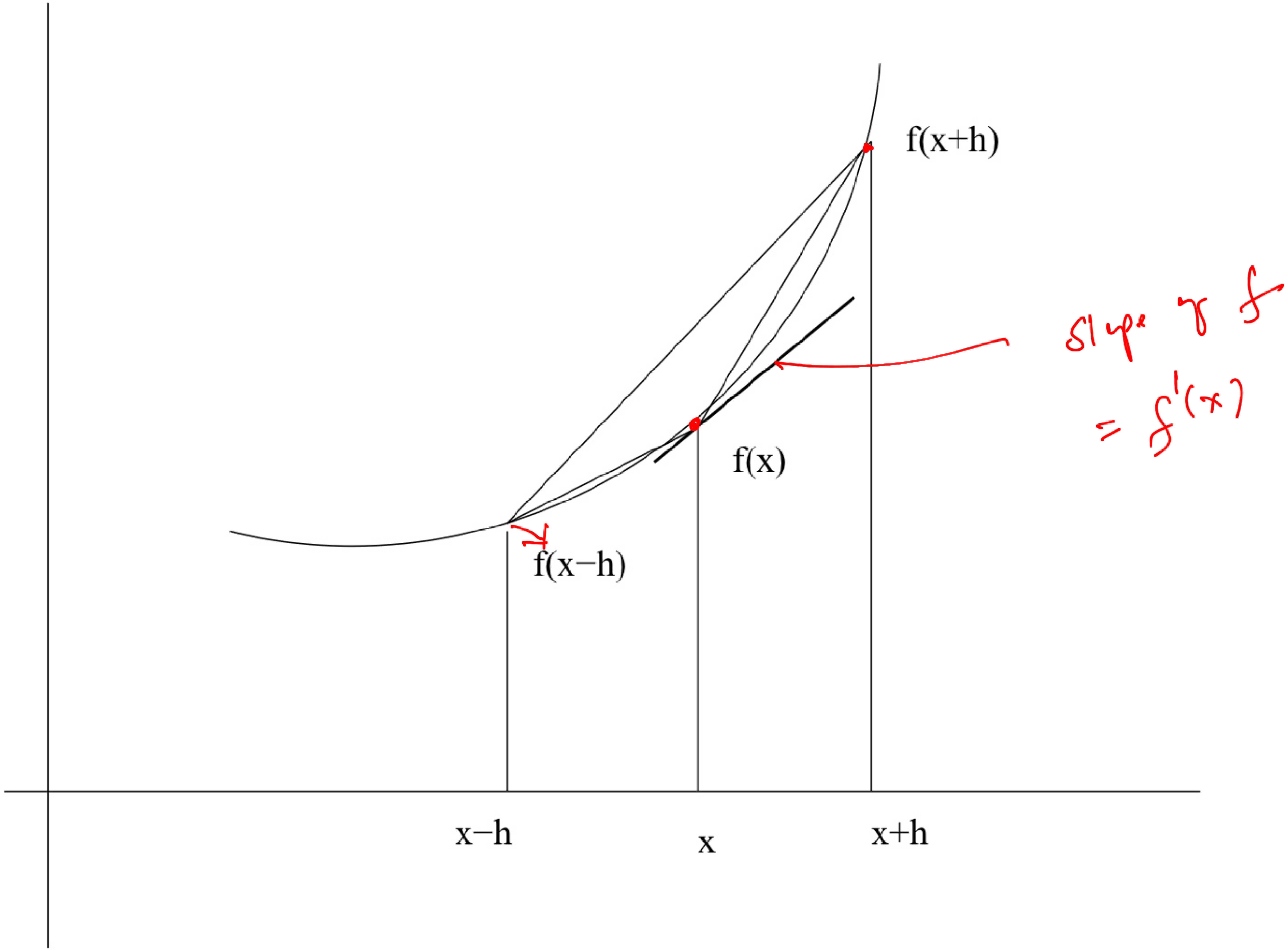
$$f'(x) \quad \approx \quad \frac{f(x+h) - f(x-h)}{2h}, \qquad (8)$$

(central difference formula)

provides a better approximation to $f'(x)$. In this case, the truncation error is

$$\textbf{T.E.} \; = O(h^2).$$

Geometrical Interpretation



An approximation to the second derivative $f''(x)$ is obtained as follows. Extending Taylor's expansion (5) and (6) by one more term, we have

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_1) \qquad (9)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_2), \qquad (10)$$

Adding (9) and (10), we obtain

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{24}f^{(4)}(\xi)$$

Exercise:

Find an approximation to $f'''(x)$ using Taylor's theorem.

for some $\xi \in (x-h, x+h)$. The formula

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \qquad (11)$$

provides an approximation to $f''(x)$. The truncation error is

$$\textbf{T.E.} = O(h^2).$$

*** End ***

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

$$- \frac{h^2}{24}\left[f^{(IV)}(\xi_1) + f^{(IV)}(\xi_2) \right]$$

If $f \in C^4([x-h, x+h])$, then $\exists\ \xi \in (x-h, x+h)$ s.t.

$$f^{(IV)}(\xi) = \frac{1}{2}\left[f^{(IV)}(\xi_1) + f^{(IV)}(\xi_2) \right]$$

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

$\xi \in (x-h, x+h)$.