# Numerical Analysis I
# Numerical Differentiation and Integration

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[1] These slides are based on Prof. Tsung-Ming Huang(NTNU)'s original slides

# Outline

# Numerical Differentiation

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

## Question

How accurate is

$$\frac{f(x_0 + h) - f(x_0)}{h}?$$

Suppose a given function $f$ has continuous first derivative and $f''$ exists. From Taylor's theorem

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

where $\xi$ is between $x$ and $x + h$, one has

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

Hence it is reasonable to use the approximation

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

which is called forward finite difference, and the error involved is

$$|e| = \frac{h}{2}|f''(\xi)| \leq \frac{h}{2} \max_{t \in (x, x+h)} |f''(t)|.$$

Similarly one can derive the backward finite difference approximation

$$f'(x) \approx \frac{f(x) - f(x-h)}{h} \tag{1}$$

which has the same order of truncation error as the forward finite difference scheme.

The forward difference is an $O(h)$ scheme. An $O(h^2)$ scheme can also be derived from the Taylor's theorem

$$\begin{aligned} f(x+h) &= f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{6}f'''(\xi_1)h^3 \\ f(x-h) &= f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{6}f'''(\xi_2)h^3, \end{aligned}$$

where $\xi_1$ is between $x$ and $x+h$ and $\xi_2$ is between $x$ and $x-h$. Hence

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{1}{6}[f'''(\xi_1) + f'''(\xi_2)]h^3$$

and

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{12}[f'''(\xi_1) + f'''(\xi_2)]h^2$$

Let

$$M = \max_{z\in[x-h,x+h]} f'''(z) \quad \text{and} \quad m = \min_{z\in[x-h,x+h]} f'''(z).$$

If $f'''$ is continuous on $[x-h, x+h]$, then by the intermediate value theorem, there exists $\xi \in [x-h, x+h]$ such that

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

Hence

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{1}{6}f'''(\xi)h^2 = \frac{f(x+h) - f(x-h)}{2h} + O(h^2).$$

This is called center difference approximation and the truncation error is

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

Similarly, we can derive an $O(h^2)$ scheme from Taylor's theorem for $f''(x)$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{1}{12}f^{(4)}(\xi)h^2,$$

where $\xi$ is between $x-h$ and $x+h$.

# Polynomial Interpolation Method

Suppose that $(x_0, f(x_0))$, $(x_1, f(x_1)) \cdots, (x_n, f(x_n))$ have been given, we apply the Lagrange polynomial interpolation scheme to derive

$$P(x) = \sum_{i=0}^{n} f(x_i) L_i(x),$$

where

$$L_i(x) = \prod_{j=0, j \neq i}^{n} \frac{x - x_j}{x_i - x_j}.$$

Since $f(x)$ can be written as

$$f(x) = \sum_{i=0}^{n} f(x_i) L(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w(x),$$

where

$$w(x) = \prod_{j=0}^{n} (x - x_j),$$

we have,

$$\begin{aligned} f'(x) &= \sum_{i=0} n f(x_i) L_i'(x) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) w'(x) \\ &+ \frac{1}{(n+1)!} w(x) \frac{d}{dx} f^{(n+1)}(\xi_x). \end{aligned}$$

Note that

$$w'(x) = \sum_{j=0}^{n} \prod_{i=0, i\neq j}^{n} (x - x_i).$$

Hence a reasonable approximation for the first derivative of $f$ is

$$f'(x) \approx \sum_{i=0}^{n} f(x_i) L_i'(x).$$

When $x = x_k$ for some $0 \leq k \leq n$,

$$w(x_k) = 0 \quad \text{and} \quad w'(x_k) = \prod_{i=0, i\neq k}^{n} (x_k - x_i).$$

Hence

$$f'(x_k) = \sum_{i=0}^{n} f(x_i) L_i'(x_k) + \frac{1}{(n+1)!} f^{(n+1)}(\xi_x) \prod_{i=0, i\neq k}^{n} (x_k - x_i), \qquad (2)$$

which is called an $(n+1)$-point formula to approximate $f'(x)$.

- Three Point Formulas

Since

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}$$

we have

$$L_0'(x) = \frac{2x - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}.$$

Similarly,

$$L_1'(x) = \frac{2x - x_0 - x_2}{(x_1-x_0)(x_1-x_2)} \quad \text{and} \quad L_2'(x) = \frac{2x - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}.$$

Hence

$$
\begin{aligned}
f'(x_j) &= f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}\right] \\
&+ f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}\right] + \frac{1}{6}f^{(3)}(\xi_j)\prod_{k=0,k\neq j}^{2}(x_j - x_k),
\end{aligned}
$$

for each $j = 0, 1, 2$. Assume that

$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h, \quad \text{for some} \quad h \neq 0.$$

Then

$$
\begin{aligned}
f'(x_0) &= \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_0), \\
f'(x_1) &= \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_2)\right] - \frac{h^2}{6}f^{(3)}(\xi_1), \\
f'(x_2) &= \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_2).
\end{aligned}
$$

That is

$$
\begin{aligned}
f'(x_0) &= \frac{1}{h}\left[-\frac{3}{2}f(x_0)+2f(x_0+h)-\frac{1}{2}f(x_0+2h)\right]+\frac{h^2}{3}f^{(3)}(\xi_0), \\
f'(x_0+h) &= \frac{1}{h}\left[-\frac{1}{2}f(x_0)+\frac{1}{2}f(x_0+2h)\right]-\frac{h^2}{6}f^{(3)}(\xi_1), \qquad (3)\\
f'(x_0+2h) &= \frac{1}{h}\left[\frac{1}{2}f(x_0)-2f(x_0+h)+\frac{3}{2}f(x_0+2h)\right]+\frac{h^2}{3}f^{(3)}(\xi_2) \qquad (4)
\end{aligned}
$$

Using the variable substitution $x_0$ for $x_0+h$ and $x_0+2h$ in (3) and (4), respectively, we have

$$
\begin{aligned}
f'(x_0) &= \frac{1}{2h}\left[-3f(x_0)+4f(x_0+h)-f(x_0+2h)\right]+\frac{h^2}{3}f^{(3)}(\xi_0), \qquad (5)\\
f'(x_0) &= \frac{1}{2h}\left[-f(x_0-h)+f(x_0+h)\right]-\frac{h^2}{6}f^{(3)}(\xi_1), \\
f'(x_0) &= \frac{1}{2h}\left[f(x_0-2h)-4f(x_0-h)+3f(x_0)\right]+\frac{h^2}{3}f^{(3)}(\xi_2). \qquad (6)
\end{aligned}
$$

Note that (6) can be obtained from (5) by replacing $h$ with $-h$.

- Five-point Formulas

$$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30} f^{(5)}(\xi),$$

where $\xi \in (x_0 - 2h, x_0 + 2h)$ and

$$f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)] + \frac{h^4}{5} f^{(5)}(\xi),$$

where $\xi \in (x_0, x_0 + 4h)$.

# Round-off Error

Consider

$$f'(x_0) = \frac{1}{2h}\left[-f(x_0-h)+f(x_0+h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

where $\frac{h^2}{6}f^{(3)}(\xi_1)$ is called truncation error. Let $\tilde{f}(x_0+h)$ and $\tilde{f}(x_0-h)$ be the computed values of $f(x_0+h)$ and $f(x_0-h)$, respectively. Then

$$f(x_0+h) = \tilde{f}(x_0+h) + e(x_0+h)$$

and

$$f(x_0-h) = \tilde{f}(x_0-h) + e(x_0-h).$$

Therefore, the total error in the approximation

$$f'(x_0) - \frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h} = \frac{e(x_0+h)-e(x_0-h)}{2h} - \frac{h^2}{6}f^{(3)}(\xi_1)$$

is due in part to round-off error and in part to truncation error.

Assume that

$$|e(x_0 \pm h)| \leq \varepsilon \quad \text{and} \quad |f^{(3)}(\xi_1)| \leq M.$$

Then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} \right| \leq \frac{\varepsilon}{h} + \frac{h^2}{6} M \equiv e(h).$$

Note that $e(h)$ attains its minimum at $h = \sqrt[3]{3\varepsilon/M}$.
In double precision arithemetics, for example, $\varepsilon \approx |f(x_0 \pm h)| \times 10^{-16}$.
The minimum is $O(\sqrt[3]{M\varepsilon^2}) = O(10^{-10})$.