

# Chapter 6 Numerical Differentiation

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## 6.1 Numerical Differentiation

### Review on the Definition of Derivative:

- The derivative of the function  $f$  at  $x_0$  is

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

- **Question:** How to approximate this number  $f'(x_0)$ ?

- Suppose  $f \in C^2[a, b]$ ,  $x_0, x_1 \in (a, b)$ .
- Let  $h = x_1 - x_0$  and is sufficiently small, thus  $x_1 = x_0 + h$ .
- Using  $(x_0, f(x_0)), (x_1, f(x_1))$ , construct linear Lagrange polynomial  $P_1(x)$ :

$$\begin{aligned}P_1(x) &= f(x_0) \frac{x - x_1}{x_0 - x_1} + f(x_1) \frac{x - x_0}{x_1 - x_0} \\&= f(x_0) \frac{x - x_0 - h}{-h} + f(x_0 + h) \frac{x - x_0}{h} \\&= f(x_0) + \frac{x - x_0}{h} (f(x_0 + h) - f(x_0)).\end{aligned}$$

- Thus

$$f(x) = P_1(x) + \frac{f''(\xi(x))}{2!} (x - x_0)(x - x_1)$$

where  $\xi(x) \in [x_0, x_1] \subset [a, b]$ .

- Differentiating this equation with respect to  $x$ , gives

$$\begin{aligned} f'(x) &= P_1'(x) + \frac{d}{dx} \left[ \frac{f''(\xi(x))}{2!} (x - x_0)(x - x_1) \right] \\ &= \frac{f(x_0 + h) - f(x_0)}{h} + \frac{2(x - x_0) - h}{2} f''(\xi(x)) \\ &\quad + \frac{(x - x_0)(x - x_0 - h)}{2} \frac{d}{dx} f''(\xi(x)) \end{aligned}$$

- Since  $h$  is sufficient small, we have

$$f'(x) \approx \frac{f(x_0 + h) - f(x_0)}{h}.$$

- For arbitrary  $x \in [x_0, x_0 + h]$ , there is no information about

$$\frac{d}{dx}f''(\xi(x)) = f^{(3)}(\xi(x))\xi'(x),$$

so the truncation error cannot be estimated.

- When  $x = x_0$ , however, the coefficient of  $\frac{d}{dx}f''(\xi(x))$  is zero, and the formula simplifies to

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2}f''(\xi). \quad (1)$$

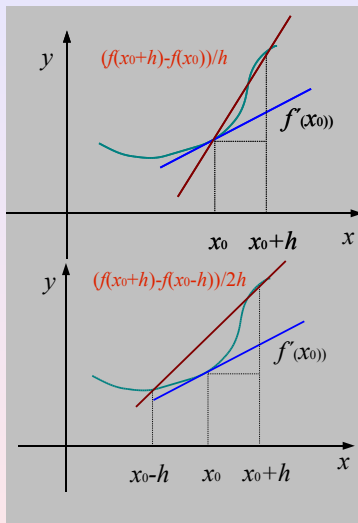
# Two useful Formulas

- **Forward-Difference Formula:**

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h},$$

- **Backward-Difference Formula:**

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h}.$$



# General Case

- Suppose  $f \in C^{(n+1)}(I)$ , and  $\{x_0, x_1, \dots, x_n\}$  are  $(n+1)$  distinct numbers in  $I$ .
- How to obtain more general derivative approximation formulas?
- From Lagrange Polynomial Interpolation method, we have

$$f(x) = \sum_{k=0}^n f(x_k) L_k(x) + \frac{(x - x_0) \cdots (x - x_n)}{(n+1)!} f^{(n+1)}(\xi(x))$$

for some  $\xi(x)$  in  $I$ , where  $L_k(x)$  denotes the  $k$ th Lagrange polynomial for  $f$  at  $x_k$ ,  $k = 0, 1, \dots, n$ .



- Differentiating this expression gives

$$\begin{aligned}
 f'(x) &= \sum_{k=0}^n f(x_k) L'_k(x) \\
 &+ \frac{d}{dx} \left[ \frac{(x - x_0) \cdots (x - x_n)}{(n+1)!} \right] f^{(n+1)}(\xi(x)) \\
 &+ \frac{(x - x_0) \cdots (x - x_n)}{(n+1)!} \frac{d}{dx} [f^{(n+1)}(\xi(x))]
 \end{aligned}$$

- Again, we have a problem estimating the truncation error **unless  $x$  is one of the numbers  $x_j$** .

# $(n + 1)$ - Point Formula

- If  $x$  is one of the numbers  $x_j$ , the term involving  $\frac{d}{dx}[f^{(n+1)}(\xi(x))]$  is zero, then we have

$$f'(x_j) = \sum_{k=0}^n f(x_k) L'_k(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{k=0, k \neq j}^n (x_j - x_k) \quad (2)$$

for  $j = 0, 1, \dots, n$

- Equation (2) is called an  $(n + 1)$ - **Point Formula** to approximate  $f'(x_j)$ ,  $j = 0, 1, \dots, n$ .

# Most common Cases: Three-point and Five-point formulas

- First we derive **Three-point formulas**:
- Since

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}, \text{ and } L'_0(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)};$$

$$L_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}, \text{ and } L'_1(x) = \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)};$$

$$L_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}, \text{ and } L'_2(x) = \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)};$$

- 由二次Lagrange 插值公式, 有

$$\begin{aligned} f(x) &= f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x) \\ &\quad + \frac{f^{(3)}(\xi)}{3!}(x-x_0)(x-x_1)(x-x_2) \end{aligned}$$

- 两端求导, 可得

$$\begin{aligned} f'(x) &= f(x_0)L'_0(x) + f(x_1)L'_1(x) + f(x_2)L'_2(x) \\ &\quad + \frac{d}{dx} \left[ \frac{f^{(3)}(\xi)}{6}(x-x_0)(x-x_1)(x-x_2) \right] \end{aligned}$$

- 取  $x = x_j$ , 得:

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

for each  $j = 0, 1, 2$ ,  $\xi_j$  depends on  $x_j$ .

# Note:

- 1 If the nodes are equally spaced, for example, let  $x_1 = x_0 + h$  and  $x_2 = x_1 + 2h$ , for some  $h \neq 0$ .
- 2 Then using Equation (3) with  $x_0 = x_0$ ,  $x_1 = x_0 + h$ , and  $x_2 = x_0 + 2h$  gives

$$\begin{aligned} f'(x_0) &= \frac{1}{h} \left[ -\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2) \right] + \frac{h^2}{3}f^{(3)}(\xi_0) \\ &= \frac{1}{2h} \left[ -3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h) \right] \\ &\quad + \frac{h^2}{3}f^{(3)}(\xi_0) \end{aligned}$$

# Note:

- ① If the nodes are equally spaced, for example, let  $x_1 = x_0 + h$  and  $x_2 = x_1 + 2h$ , for some  $h \neq 0$ .
- ② Then using Equation (3) with  $x_0 = x_0$ ,  $x_1 = x_0 + h$ , and  $x_2 = x_0 + 2h$  gives

$$\begin{aligned} f'(x_0) &= \frac{1}{h} \left[ -\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2) \right] + \frac{h^2}{3}f^{(3)}(\xi_0) \\ &= \frac{1}{2h} \left[ -3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h) \right] \\ &\quad + \frac{h^2}{3}f^{(3)}(\xi_0) \end{aligned}$$

$$\begin{aligned}
 f'(x_0 + h) &= f'(x_1) \\
 &= \frac{1}{2h} \left[ -f(x_0) + f(x_0 + 2h) \right] - \frac{h^2}{6} f^{(3)}(\xi_1), \\
 f'(x_0 + 2h) &= f'(x_2) \\
 &= \frac{1}{2h} \left[ f(x_0) - 4f(x_1) + 3f(x_2) \right] + \frac{h^2}{3} f^{(3)}(\xi_2).
 \end{aligned}$$

- Using variable substitution  $x_0$ , the formula to an approximation for  $f'(x_0)$  can be changed.
- Take nodes as  $x_0, x_0 + h, x_0 + 2h$ , then

$$f'(x_0) = \frac{1}{2h} \left[ -3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h) \right] + \frac{h^2}{3} f^{(3)}(\xi_0).$$

- Take nodes as  $x_0 - h, x_0, x_0 + h$ , then

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

- Take nodes as  $x_0 - 2h, x_0 - h, x_0$ , then

$$f'(x_0) = \frac{1}{2h} \left[ f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0) \right] + \frac{h^2}{3} f^{(3)}(\xi_2).$$



- Note that since the last of these equations can be obtained from the first by simply replacing  $h$  with  $-h$ , there are actually only two formulas.
- First formulas

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}(\xi_0), \quad (3)$$

where  $\xi_0$  lies between  $x_0$  and  $x_0 + 2h$

- Second formulas

$$f'(x_0) = \frac{1}{2h}[-f(x_0 - h) + f(x_0 + h)] - \frac{h^2}{6}f^{(3)}(\xi_1), \quad (4)$$

where  $\xi_1$  lies between  $(x_0 - h)$  and  $(x_0 + h)$ .

- The error in Eq.(4) is approximately half the error in Eq.(3).
- This is because Eq.(4) uses data on both sides of  $x_0$ . and Eq.(3) uses data on only one side.
- Note also that  $f$  needs to be evaluated at only two points in Eq.(4). whereas in Eq.(3) three evaluations are needed.
- The methods presented in Eqs.(4) and (3) are called **three-point formulas** (even though the third point  $f(x_0)$  does not appear in Eq.(4).

- Similarly, there are methods known as **five-point formulas** that involve evaluating the function at  $x_0 - 2h, x_0 - h, x_0, x_0 + h, x_0 + 2h$ .

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

- Particularly with regard to the clamped cubic spline interpolation, is

$$f'(x_0) = \frac{1}{12h} [-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5} f^{(5)}(\xi) \quad (6)$$

where  $\xi$  lies between  $x_0$  and  $x_0 + 4h$ .

# Methods to derive higher derivatives of a function

- By Taylor polynomial, we have

$$\begin{aligned}f(x_0 + h) &= f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 \\&\quad + \frac{1}{6}f^{(3)}(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4\end{aligned}$$

$$\begin{aligned}f(x_0 - h) &= f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 \\&\quad - \frac{1}{6}f^{(3)}(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_{-1})h^4\end{aligned}$$

where  $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$ .

- If we add this two equations, we can get

$$\begin{aligned}f(x_0 + h) + f(x_0 - h) &= 2f(x_0) + f''(x_0)h^2 \\&\quad + \frac{h^4}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})].\end{aligned}$$

- Suppose  $f^{(4)}$  is continuous, thus there exists  $\xi \in [x_0 - h, x_0 + h]$ , such that

$$f^{(4)}(\xi) = \frac{1}{2}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]$$

- Rewrite above formula as

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

# 误差分析

- Take above formula as an example:

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

- 在实际计算中，通常还要考虑观测数据本身的随机系统误差和舍入误差，同时还要考虑计算格式设计本身的截断误差，如 $f''(x_0)$ 的上述计算格式，总误差为

$$E(f, h) \leq \frac{4\varepsilon}{h^2} + \frac{Mh^4}{12}$$

- To minimize the total error  $E(f, h)$ , we can choose  $h$  as:  
Suppose  $g(h) = \frac{4\varepsilon}{h^2} + \frac{Mh^4}{12}$ , and let

$$g'(h) = -\frac{8\varepsilon}{h^3} + \frac{Mh}{6} = 0,$$

gives

$$h = \left(\frac{48\varepsilon}{M}\right)^{1/4}$$

## 6.2 Richardson's Extrapolation

- Richardson's Extrapolation is used to generate high-accuracy results while using low-order formulas.
- Extrapolation can be applied whenever it is known that the approximation technique has an error term with a predictable form, one that depends on a parameter, usually the step size  $h$ .
- Suppose that for each number  $h \neq 0$  we have a formula  $N(h)$  that approximates an unknown value  $M$  and that the truncation error involved with the approximation has the form

$$M - N(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots$$

for some collection of unknown, but nonzero, constants  $K_1, K_2, K_3, \dots$

- To see specifically how we can generate these higher-order formulas, let us consider the formula for approximating  $M$  of the form

$$M = N(h) + K_1h + K_2h^2 + K_3h^3 + \cdots \quad (7)$$

- Since the formula is assumed to hold for all positive  $h$ , consider the result when we replace the parameter  $h$  by half its value.
- Then we have the formula

$$M = N\left(\frac{h}{2}\right) + K_1\frac{h}{2} + K_2\frac{h^2}{4} + K_3\frac{h^3}{8} + \cdots \quad (8)$$



- Subtracting (7) from twice this equation eliminates the term involving  $K_1$  and gives

$$M = [N(\frac{h}{2}) + (N(\frac{h}{2}) - N(h))] + \\ + K_2(\frac{h^2}{2} - h^2) + K_3(\frac{h^3}{4} - h^3) + \dots$$

- To facilitate the discussion, we define  $N_1(h) \equiv N(h)$  and

$$N_2(h) = N_1(\frac{h}{2}) + [N_1(\frac{h}{2}) - N_1(h)] \quad (9)$$

- Then we have the  $O(h^2)$  approximation formula for  $M$ :

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 + \dots \quad (10)$$

- If we now replace  $h$  by  $\frac{h}{2}$  in this formula, we have

$$M = N_2\left(\frac{h}{2}\right) - \frac{K_2}{8}h^2 - \frac{3K_3}{32}h^3 - \dots \quad (11)$$

- This can be combined with Eq.(9) to eliminate the  $h^2$  term. Specifically, subtracting (10) from 4 times Eq. (11) gives

$$3M = 4N_2\left(\frac{h}{2}\right) - N_2(h) + \frac{3K_3}{8}h^3 + \dots \quad (12)$$

- Which simplifies to the  $O(h^3)$  formula for approximating  $M$ :

$$M = \left[ N_2\left(\frac{h}{2}\right) + \frac{N_2(h/2) - N_2(h)}{3} \right] + \frac{K_3}{8}h^3 + \dots \quad (13)$$

- By defining

$$N_3(h) \equiv N_2\left(\frac{h}{2}\right) + \frac{N_2(h/2) - N_2(h)}{3},$$

- we have the  $O(h^3)$  formula:

$$M = N_3(h) + \frac{K_3}{8}h^3 + \dots$$

- The process is continued by constructing the  $O(h^4)$  approximation

$$N_4(h) = N_3\left(\frac{h}{2}\right) + \frac{N_3(h/2) - N_3(h)}{7}, \quad (14)$$

- the  $O(h^5)$  approximation

$$N_5(h) = N_4\left(\frac{h}{2}\right) + \frac{N_4(h/2) - N_4(h)}{15}, \quad (15)$$

and so on.

- In general, if  $M$  can be written in the form

$$M = N(h) + \sum_{j=1}^{m-1} K_j h^j + O(h^m),$$

then for each  $j = 2, 3, \dots, m$ , we have an  $O(h^j)$  approximation of the form

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1}. \quad (16)$$

# APPLICATION:

- Suppose we expand the function  $f$  in a fourth Taylor polynomial about  $x_0$ .
- Then

$$\begin{aligned}f(x) = & f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2 \\& + \frac{1}{6}f^{(3)}(x_0)(x - x_0)^3 + \frac{1}{24}f^{(4)}(x_0)(x - x_0)^4 \\& + \frac{1}{120}f^{(5)}(\xi)(x - x_0)^5\end{aligned}$$

for some number  $\xi$  between  $x$  and  $x_0$ .

Evaluating  $f$  at  $x_0 + h$  and  $x_0 - h$  gives

$$\begin{aligned} f(x_0 + h) = & f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f^{(3)}(x_0)h^3 + \\ & + \frac{1}{24}f^{(4)}(x_0)h^4 + \frac{1}{120}f^{(5)}(\xi_1)h^5 \end{aligned} \quad (17)$$

and

$$\begin{aligned} f(x_0 - h) = & f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f^{(3)}(x_0)h^3 + \\ & + \frac{1}{24}f^{(4)}(x_0)h^4 - \frac{1}{120}f^{(5)}(\xi_2)h^5 \end{aligned} \quad (18)$$

where  $x_0 - h < \xi_2 < x_0 < \xi_1 < x_0 + h$ .

- Subtracting Eq.(17) from Eq.(18)

$$f(x_0 + h) - f(x_0 - h) = 2hf'(x_0) + \frac{h^3}{3}f^{(3)}(x_0) + \frac{h^5}{120}[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)]. \quad (19)$$

- If  $f^{(5)}$  is continuous on  $[x_0 - h, x_0 + h]$ , the Intermediate Value Theorem implies that a number  $\tilde{\xi}$  in  $(x_0 - h, x_0 + h)$  exists with

$$f^{(5)}(\tilde{\xi}) = \frac{1}{2}[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)].$$

- As a consequence, Eq.(19) can be solved for  $f'(x_0)$  to give the  $O(h^2)$  approximation

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6}f^{(3)}(x_0) - \frac{h^4}{120}f^{(5)}(\tilde{\xi}) \quad (20)$$

- Although the approximation in Eq.(20) is the same as that given in the three-point formula in Eq.(4).
- The unknown evaluation point occurs now in  $f^{(5)}$ , rather than in  $f^{(3)}$ .



- Extrapolation takes advantage of this by first replacing  $h$  in Eq.(20) with  $2h$  to give the new formula

$$f'(x_0) = \frac{1}{4h}[f(x_0 + 2h) - f(x_0 - 2h)] - \frac{4h^2}{6}f^{(3)}(x_0) - \frac{16h^4}{120}f^{(5)}(\hat{\xi}), \quad (21)$$

where  $\hat{\xi}$  is between  $x_0 - 2h$  and  $x_0 + 2h$ .

- Multiplying Eq.(20) by 4 and subtracting Eq.(21) produces

$$3f'(x_0) = \frac{2}{h}[f(x_0 + h) - f(x_0 - h)] - \frac{1}{4h}[f(x_0 + 2h) - f(x_0 - 2h)] - \frac{h^4}{30}f^{(5)}(\tilde{\xi}) + \frac{2h^4}{15}f^{(5)}(\hat{\xi}) \quad (22)$$

- If  $f^{(5)}(x_0)$  is continuous on  $[x_0 - 2h, x_0 + 2h]$
- An alternative method can be used to show that  $f^{(5)}(\hat{\xi})$  and  $f^{(5)}(\tilde{\xi})$  can be replaced by a common value  $f^{(5)}(\hat{\xi})$ .
- Using this result and dividing by 3 produces the five-point formula

$$f'(x_0) = \frac{1}{12h} [f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30} f^{(5)}(\xi) \quad (23)$$

which is the five-point formula given as Eq.(5).



