Chapter 4 Numerical Differentiation

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Review on the Definition of Derivative:

- The derivative of the function f at x_0 is

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

- **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

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

- Since h is sufficient small, we have

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

Notes:

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

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

  so the truncation error cannot be estimated.
- When $x = x_0$, however, the coefficient of $\frac{\mathrm{d}}{\mathrm{d}x} f''(\xi(x))$ is zero, and the formula simplifies to

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

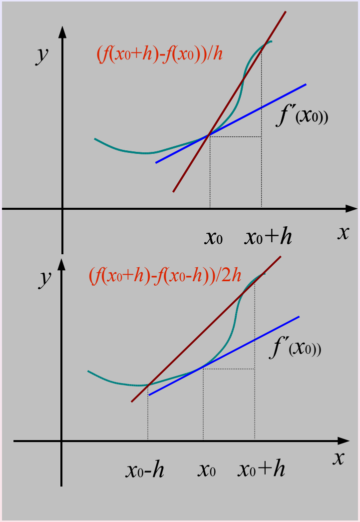
Two useful Formulas

- **Forward-Difference Formula:**

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

- **Backward-Difference Formula:**

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


y
(f(x0+h)-f(x0))/h
f′(x0))
x0
x0+h
x
y
(f(x0+h)-f(x0-h))/2h
f′(x0))
x0-h
x0
x0+h
x

General Case

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

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

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

- Differentiating this expression gives

$$
\begin{aligned}
f'(x) = &\sum_{k=0}^{n} f(x_k) L_k'(x) \\
&\quad + \frac{\mathrm{d}}{\mathrm{d}x}\Big[\frac{(x-x_0)\cdots(x-x_n)}{(n+1)!}\Big] f^{(n+1)}(\xi(x)) \\
&\quad\quad + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} \frac{\mathrm{d}}{\mathrm{d}x}[f^{(n+1)}(\xi(x))]
\end{aligned}
$$

- 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 $\frac{\mathrm{d}}{\mathrm{d}x}[f^{(n+1)}(\xi(x))]$ is zero, then we have

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

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

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

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

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

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

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

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

- 由二次Lagrange 插值公式，有

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

- 两端求导，可得

$$\begin{aligned} f'(x) &= f(x_0)L_0'(x) + f(x_1)L_1'(x) + f(x_2)L_2'(x) \\ &+ \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{f^{(3)}(\xi)}{6}(x-x_0)(x-x_1)(x-x_2)\right] \end{aligned}$$

- 取 $x = x_j$, 得:

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

for each $j = 0, 1, 2$, ξ_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 $x_2 = x_0 + 2h$, and let $x = x_0$, gives

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

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- let $x = x_1$, gives:

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

- let $x = x_2$, gives

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

- 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

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

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

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

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

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

- 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

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

  where ξ_0 lies between x_0 and $x_0 + 2h$
- Second formulas

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

  where ξ_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 $x_0 - 2h, x_0 - h, x_0, x_0 + h, x_0 + 2h$.

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

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

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

where ξ lies between x_0 and $x_0 + 4h$.

Methods to derive higher derivatives of a function

- By Taylor polynomial, we have

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

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

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

4.2 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 $K_1, K_2, K_3, \ldots$

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

$$M = N(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots \tag{7}$$

- 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

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

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

$$\begin{aligned} M &= [N(\frac{h}{2}) + (N(\frac{h}{2}) - N(h))] + \\ &\quad + K_2(\frac{h^2}{2} - h^2) + K_3(\frac{h^3}{4} - h^3) + \cdots . \end{aligned}$$

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

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

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

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

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

$$M = N_2(\frac{h}{2}) - \frac{K_2}{8}h^2 - \frac{3K_3}{32}h^3 - \cdots \qquad (11)$$

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

$$3M = 4N_2(\frac{h}{2}) - N_2(h) + \frac{3K_3}{8}h^3 + \cdots \qquad (12)$$

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

$$M = [N_2(\frac{h}{2}) + \frac{N_2(h/2) - N_2(h)}{3}] + \frac{K_3}{8}h^3 + \cdots \qquad (13)$$

- By defining

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

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

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

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

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

- the $O(h^5)$ approximation

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

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 $j = 2, 3, ..., m$, we have an $O(h^j)$ approximation of the form

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

APPLICATION:

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

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

for some number ξ between x and x_0.

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

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

and

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

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

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

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

- 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

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

- 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

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

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

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

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

- 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 he five-point formula

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

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