Chapter 2 Numerical Differentiation

- **Forward/Backward Difference**
- **Central Difference**
- **Richardson Extrapolation**

- **Definition**

If the following limit exists

$$\lim_{h\to 0}\frac{f(x+h)-f(x)}{h}\equiv f^{'}(x)\ , \tag{1}$$

then we call it the derivative of function $f(x)$.

How to calculate $f^{'}(x)$ numerically with *finite* h?

- **Naive Formula**

$$D_h f(x)\equiv\frac{f(x+h)-f(x)}{h}\ ,$$

with small h.

Use Taylor expansion

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

$$f^{'}(x)-D_h f(x)=-\frac{h}{2}\left(f^{''}(x)+\cdots\right)=-\frac{h}{2}f^{''}(c)\ . \tag{3}$$

So the error is proportional to h.

This is also called *forward difference* approximation.

By symmetry, we have *backward difference* approximation

$$D_h f(x)\equiv\frac{f(x-h)-f(x)}{h}\ . \tag{4}$$

- **Central Difference Formula**

  By Taylor expansion

$$\begin{aligned} f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2!}f''(x) \\ &+ \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{iv}(x) + \cdots \quad (5) \\ f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2!}f''(x) \\ &- \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{iv}(x) - \cdots \quad (6) \end{aligned}$$

$$f(x+h) - f(x-h) = 2hf'(x) + 2\frac{h^3}{3!}f'''(x) + \cdots \quad (7)$$

$$D_h f(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)\ . \quad (8)$$

As a general rule, symmetric expressions are more accurate than nonsymmetric ones.

Similarly, we obtain

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)\ . \quad (9)$$

However,

$$f''(x) = \frac{f(x) - 2f(x+h) + f(x+2h)}{h^2} + O(h)\ . \quad (10)$$

- **Richardson Extrapolation**

  Again, let's write

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(x) + \cdots \quad (11)$$

  $h \to 2h$

$$f'(x) = \frac{f(x+2h) - f(x-2h)}{4h} - \frac{4h^2}{6} f'''(x) + \cdots \quad (12)$$

  Do 4 × Eq. (**??**) - Eq. (**??**), we get

$$f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h},$$

  with error

$$E(h) = \frac{h^4}{30} f^{v}(x) + \cdots \ .$$

  Similarly,

$$f''(x) = \frac{1}{12h^2} \quad (-f(x-2h) + 16f(x-h) - 30f(x) \\ +16f(x+h) - f(x+2h)) + O(h^4) \ .$$

  $\vdots$.

  These expressions can become cumbersome!

Let $D_1(h)$ be the approximation to the derivative obtained from the 3-point central difference formula with step size h. Because the error is the order of h^2, $D_1(2h)$ should have about 4 times the error of $D_1(h)$. Thus

$$-O(h^2) = \frac{D_1(2h) - D_1(h)}{2^2 - 1} \,. \tag{13}$$

Construct a better approximation by subtracting $-O(h^2)$ from $D_1(h)$:

$$\begin{aligned} D_2(h) &= D_1(h) - \frac{D_1(2h) - D_1(h)}{2^2 - 1} \\ &= \frac{4D_1(h) - D_1(2h)}{2^2 - 1} \end{aligned} \tag{14}$$

Similarly, $D_2(h)$ contains error of h^4 so $D_2(2h)$ contains 2^4 times as much error as $D_2(h)$, and we have

$$\begin{aligned} D_3(h) &= D_2(h) - \frac{D_2(2h) - D_2(h)}{2^4 - 1} \\ &= \frac{16D_2(h) - D_2(2h)}{2^4 - 1} \end{aligned} \tag{15}$$

Continue this processes: $(f'(x) = \lim_{i\to\infty} D_i(h))$

$$\begin{aligned} D_{i+1}(h) &= D_i(h) - \frac{D_i(2h) - D_i(h)}{2^{2i} - 1} \\ &= \frac{2^{2i}D_i(h) - D_i(2h)}{2^{2i} - 1} \end{aligned} \tag{16}$$

Example 1. $f'(x)$ for $f(x) = \cos(x)$ at $x = \pi/6$.

(Exact answer is $f'(\pi/6) = 0.5$)

h	$D_h f$	Error	Ratio
0.1	-0.54243	0.04243	
0.05	-0.52144	0.02144	1.98
0.025	-0.51077	0.01077	1.99
0.0125	-0.50540	0.00540	1.99
0.00625	-0.50270	0.00270	2.00
0.003125	-0.50135	0.00135	2.00

(forward)

0.1	-0.49916708	0.0008329	
0.05	-0.49979169	0.0002083	4.00
0.025	-0.49994792	0.0000521	4.00
0.0125	-0.49998698	0.0000130	4.00
0.00625	-0.49999674	0.0000033	4.00

(central)

Example 2. $f''(x)$ for $f(x) = \cos(x)$ at $x = \pi/6$.

(Exact answer is $f''(\pi/6) = -0.86602540$)

h	$D_h^{(2)} f$	Error	Ratio
0.5	-0.84813289	-1.789E-2	
0.25	-0.86152424	-4.501E-3	3.97
0.125	-0.86489835	-1.127E-3	3.99
0.0625	-0.86574353	-2.819E-4	4.00
0.03125	-0.86595493	-7.048E-5	4.00

(central)

Example 3. $f'(x)$ for $f(x) = xe^x$ at $x = 2$.

(Exact answer is $f'(2) = 3e^2 = 22.16176\ 82968$.

h	D_1	D_2	D_3	D_4
0.4	23.16346 42931			
0.2	22.41416 06570	22.16439 27783		
0.1	22.22878 68803	22.16699 56214	22.16716 91443	
0.05	22.18256 48578	22.16715 75170	22.16716 83100	22.16716 82968

Example 2'. $f''(x)$ for $f(x) = \cos(x)$ at $x = \pi/6$.

(Exact answer is $f''(\pi/6) = -0.86602540$)

h	$D_h^{(2)}f$	Error
0.5000000	-0.8481328	0.0178925
0.2500000	-0.8615236	0.0045018
0.1250000	-0.8648949	0.0011305
0.0625000	-0.8657379	0.0002875
0.0312500	-0.8659058	0.0001196
0.0156250	-0.8659668	0.0000586
0.0078125	-0.8662109	-0.0001855
0.0039062	-0.8671875	-0.0011621

(*central*)

- **Effects of Error in Function Values**

  Recall

$$f''(x_1) = \frac{f(x_2) - 2f(x_1) + f(x_0)}{h^2} \ ,$$

  for $x_2 = x_1 + h$ and $x_0 = x_1 - h$. There are errors in evaluating function values,

$$\epsilon_i = f(x_i) - \overline{f_i} \ , \qquad i = 0, 1, 2 \ .$$

  Thus (see Eq. (**??**))

$$f''(x_1) - \overline{f''(x_1)} = -\frac{h^2}{12} f^{(4)}(x_1) + \frac{\epsilon_2 - 2\epsilon_1 + \epsilon_0}{h^2} \ .$$

  What is the error bound and maximum steplength h?

Chapter 2 Review

Numerical Differentiation Could be Tricky!

– Forward/Backward/Central Difference

– Richardson Extrapolation

– Errors!

See example programs in the book.

- **Partial Differentiation**

  E&M: Laplace's equation.

  QM: Schödinger equation.