Chapter 6 : Numerical Differentiation:

Thm: Centered difference formula of order $O(h^2)$:

Assume that $f \in C^3[a,b]$ and that

$x-h,\ x,\ x+h \in [a,b]$, then:

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

where $E_{trun}(f,h) = \dfrac{-h^2 f^{(3)}(c)}{6} = O(h^2)$

$E_{trun}(f,h)$ is called truncation error.

Example:

x	2	3	4	5	6
y	-1	2	2	-2	4

If $h=1$, $f'(4) = \dfrac{f(5) - f(3)}{(2)(1)} = \dfrac{-2-2}{2} = -2$

If $h=2$, $f'(4) = \dfrac{f(6) - f(2)}{(2)(2)} = \dfrac{4+1}{4} = \dfrac{5}{4}$

Note that with centered difference formula, we

Can't Find $f'(2)$ & $f'(6)$.

To find $f'(2)$, we need a Forward formula

and to find $f'(6)$, we need a Backward formula

Thm: Forward and Backward Formulas of $O(h^2)$.

Forward: $$f'(x_0) = \frac{-3f_0 + 4f_1 - f_2}{2h} + \frac{h^2}{3} f^{(3)}(c)$$

Backward: $$f'(x_0) = \frac{3f_0 - 4f_{-1} + f_{-2}}{2h} + \frac{h^2}{3} f^{(3)}(c)$$

where $f_i = f(x_i) = f(x_0 + ih)$, $i = -2, -1, 0, 1, 2$

Example: In the previous table:

$$h=1, \quad f'(2) \approx \frac{-3f(2) + 4f(3) - f(4)}{2(1)} = \frac{3 + 4(2) - 2}{2} = \frac{9}{2}$$

$$h=2, \quad f'(2) \approx \frac{-3f(2) + 4f(4) - f(6)}{2(2)} = \frac{3 + 4(2) - 4}{4} = \frac{7}{4}$$

Backward for $f'(6)$

If $h=1$, $$f'(6) \approx \frac{3f(6) - 4f(5) + f(4)}{2(1)} = \frac{3(4) - 4(-2) + 2}{2}$$

If $h=2$, $$f'(6) \approx \frac{3f(6) - 4f(4) + f(2)}{2(2)} = \frac{3(4) - 4(2) + -1}{4}$$

proof: CDF of $O(h^2)$:

Start with second taylor degree poly. then

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(c)$$

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(c)$$

Now $f(x+h) - f(x-h) = 2h f'(x) + \frac{2h^3}{3!} f'''(c)$

solve it for $f'(x)$ then:

$$\frac{f(x+h) - f(x-h)}{2h} - \frac{\frac{2h^3}{3!} f'''(c)}{2h} = f'(x)$$

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

Another proof.

~~proof: CDF of $O(h^2)$; Use Newton polynomial~~

~~Let $\overset{x_0}{x-h}, \overset{x_1}{x}, \overset{x_2}{x+h} \in [a,b]$, then:~~

~~$P_2(x) = a_0 + a_1(x - x_0) + a_2(x-x_0)(x-x_1)$~~

~~$P_2'(x) = a_1 + a_2[(x-x_0) + (x-x_1)]$~~

~~Now: $a_1 = f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$~~

Proof of BDF of $O(h^2)$ Using Taylor expansion.

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f^{(3)}(c)$$

$$f(x-2h) = f(x) - 2h f'(x) + \frac{4h^2}{2!} f''(x) - \frac{8h^3}{3!} f^{(3)}(c)$$

$$-4 f_{-1} + f_{-2} = -3 f_0 + 2h f'(x) - \frac{4h^3}{3!} f^{(3)}(c)$$

$$\Rightarrow \quad f'(x) = \frac{3f_0 - 4 f_{-1} + f_{-2}}{2h} + \frac{h^3 f^{(3)}(c)}{3}.$$

Example: Derive The BDF of $O(h^2)$ Using Newton polynomial.

Let $\underbrace{x_0 - 2h}_{t_0}, \underbrace{x_0 - h}_{t_1}, \underbrace{x_0}_{t_2} \in [a,b]$

$$P_2(t) = a_0 + a_1(t-t_0) + a_2(t-t_0)(t-t_1)$$

$$P_2'(t) = a_1 + a_2\left((t-t_0)+(t-t_1)\right)$$

$$P_2'(x_0) = a_1 + a_2(2h + h) = a_1 + 3h a_2.$$

$$a_1 = \frac{f(t_1) - f(t_0)}{t_1 - t_0} = \frac{f_{-1} - f_{-2}}{h}$$

Now: $a_2 = f[t_0, t_1, t_2] =$

$$= \frac{\dfrac{f_0 - f_{-1}}{h} - \dfrac{f_{-1} - f_{-2}}{h}}{2h}$$

$$a_2 = \frac{f_0 - 2f_{-1} + f_{-2}}{2h^2}$$

$$\Rightarrow P_2'(x_0) = \frac{f_{-1} - f_{-2}}{h} + \left(\frac{f_0 - 2f_{-1} + f_{-2}}{2h^2}\right)(3h)$$

$$= \frac{2f_{-1} - 2f_{-2} + 3f_0 - 6f_{-1} + 3f_{-2}}{2h}$$

$$= \frac{3f_0 - 4f_{-1} + f_{-2}}{2h}$$

<u>Example:</u> Let $f(x) = \cos x$, $h = 0.01$ Approximate $f'(0.8)$.

[Exact = -0.7[illegible]

1) CDF of $O(h^2)$: $f'(0.8) \approx \dfrac{f(0.81) - f(0.79)}{2(0.01)}$

$f'(0.8) \approx \dfrac{\cos 0.81 - \cos 0.79}{0.02} = -0.717344135$

2) FDF of $O(h^2)$: $f'(0.8) \approx \dfrac{-3\cos(0.8) + 4\cos(0.81) - \cos(0.82)}{0.02}$

$\Rightarrow f'(0.8) \approx -0.71738017$

3) BDF of $O(h^2)$ $\quad f'(0.8) \approx \dfrac{3\cos(0.8) - 4\cos(0.79) + \cos(0.78)}{2(0.01)}$

$f'(0.8) \approx \boxed{-0.71739827}$

Example: Derive a formula to approximate $f'(x)$ using the nodes $x, x+h$.

(one point different from x, then the formula is of $O(h^1)$)

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

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

~~**Summary:** The order of the formula depends on the number of the given points different from x~~

~~**Thm:** Centered difference formula of $O(h^4)$:~~

~~Assume that $f \in C^5[a,b]$ and:~~

~~$x-2h, x-h, x, x+h, x+2h \in [a,b]$~~

~~then:~~

$$f'(x) = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h} + \underbrace{\frac{h^4 f^{(5)}(c)}{30}}_{E_{trun}(f,h) = O(h^4)}$$

Example: Let $f(x) = \cos x$, approximate $f'(0.8)$, $h = 0.01$

$$f'(0.8) \approx \frac{-f(0.82) + 8f(0.81) - 8f(0.79) + f(0.78)}{12(0.01)}$$

$$\approx -0.717356108$$

Exact: $f'(0.8) = -0.717356091$ (7 significant digits)

$\Rightarrow$ error $= C(0.01)^4 = C(10^{-8})$

6.2 High order derivation:

Thm: Centered Difference formula of order $O(h^2)$

$$f''(x) = \frac{f_1 - 2f_0 + f_{-1}}{h^2} - \underbrace{\frac{h^2}{12} f^{(4)}(c)}_{E_{tru}(f,h)}.$$

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proof:
$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f^{(3)}(x) + \frac{h^4}{4!} f^{(4)}(c)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f^{(3)}(x) + \frac{h^4}{4!} f^{(4)}(c)$$

$$\Rightarrow f_1 + f_{-1} = 2f_0 + h^2 f''(x) + \frac{h^4}{12} f^{(4)}(c)$$

$$\Rightarrow f''(x) = \frac{f_1 - 2f_0 + f_{-1}}{h^2} - \frac{h^2}{12} f^{(4)}(c).$$

Example: Let $f(x) = \cos x$, Approximate $f''(0.8)$ with $h = 0.01$ using formula of $O(h^2)$.

$$f''(0.8) \approx \frac{\cos(0.81) - 2\cos(0.8) + \cos(0.79)}{(0.01)^2}$$

$$\approx -0.69669000.$$

Thm: Centered Difference formula of $O(h^4)$

$$f''(x) = \frac{-f_2 + 16 f_1 - 30 f_0 + 16 f_{-1} - f_{-2}}{12 h^2} + \frac{h^4 f^{(6)}(c)}{90}.$$

Example: Let $f(x) = \cos x$, Approximate $f''(0.8)$ with $h = 0.01$ using formula of order $O(h^4)$

$$f''(0.8) \approx \frac{-f(0.82) + 16 f(0.81) - 30 f(0.8) + 16 f(0.79) - f(0.78)}{12(0.01)^2}$$

$$\approx -0.696705958.$$