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PHYS 512
Assignment 1
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Due 18/9/20 4:00 PM

1. a. Given known values for $f(x \pm \delta)$ and $f(x \pm 2\delta)$, estimate $f'(x)$:

→ Taylor's Theorem: $f(w) = f(w_0) + (w-w_0)f'(w_0) + (w-w_0)^2 f''(w_0)\frac{1}{2!} + \cdots$
→ letting $w_0 \to x$ and $w \to (x+\delta), (x-\delta), (x+2\delta), (x-2\delta)$ for the next 4 expansions respectively:

$$f(x+\delta) = f(x) + \delta f'(x) + \frac{1}{2!}\delta^2 f''(x) + \frac{1}{3!}\delta^3 f'''(x) + \cdots \quad (1)$$
$$f(x-\delta) = f(x) - \delta f'(x) + \frac{1}{2!}\delta^2 f''(x) - \frac{1}{3!}\delta^3 f'''(x) + \cdots \quad (2)$$
$$f(x+2\delta) = f(x) + 2\delta f'(x) + \frac{1}{2!}4\delta^2 f''(x) + \frac{1}{3!}8\delta^3 f'''(x) + \cdots \quad (3)$$
$$f(x-2\delta) = f(x) - 2\delta f'(x) + \frac{1}{2!}4\delta^2 f''(x) - \frac{1}{3!}8\delta^3 f'''(x) + \cdots \quad (4)$$

$$(1) \Rightarrow f = f(x+\delta) - \delta f' - \frac{1}{2!}\delta^2 f'' - \frac{1}{3!}\delta^3 f''' - \frac{1}{4!}\delta^4 f^{IV} - \frac{1}{5!}\delta^5 f^{V} - \cdots \quad (5)$$
$$(2) \Rightarrow \delta f' = -f(x-\delta) + f + \frac{1}{2!}\delta^2 f'' - \frac{1}{3!}\delta^3 f''' + \frac{1}{4!}\delta^4 f^{IV} - \frac{1}{5!}\delta^5 f^{V} + \cdots \quad (6)$$
$$(5) \to (6) \Rightarrow 2\delta f' = f(x+\delta) - f(x-\delta) - \frac{2}{3!}\delta^3 f''' - \frac{2}{5!}\delta^5 f^{V} - \frac{2}{7!}\delta^7 f^{VII} - \cdots \quad (7)$$
$$(7) \Rightarrow \delta f' = \tfrac{1}{2}[f(x+\delta) - f(x-\delta)] - \frac{1}{3!}\delta^3 f''' - \frac{1}{5!}\delta^5 f^{V} - \frac{1}{7!}\delta^7 f^{VII} - \cdots \quad (8)$$

$$(3) - (4) \Rightarrow f(x+2\delta) - f(x-2\delta) = \frac{4}{1!}\delta f' + \frac{16}{3!}\delta^3 f''' + \frac{64}{5!}\delta^5 f^{V} + \frac{256}{7!}\delta^7 f^{VII} + \cdots \quad (9)$$
$$(9) \Rightarrow \frac{1}{3!}\delta^3 f''' = \frac{1}{16}[f(x+2\delta) - f(x-2\delta)] - \tfrac{1}{4}\delta f' - \frac{4}{5!}\delta^5 f^{V} - \frac{16}{7!}\delta^7 f^{VII} - \cdots \quad (10)$$

$$(8) \to (10) \Rightarrow \delta f' = \tfrac{1}{2}[f(x+\delta) - f(x-\delta)] + \frac{1}{16}[f(x-2\delta) - f(x+2\delta)] + \frac{1}{4}\delta f' + \frac{3}{5!}\delta^5 f^{V} + \cdots \quad (11)$$
$$(11) \Rightarrow 3\delta f' = 2[f(x+\delta) - f(x-\delta)] + \frac{1}{4}[f(x-2\delta) - f(x+2\delta)] + \frac{12}{5!}\delta^5 f^{V}(x) + \cdots \quad (12)$$

$$(12) \Rightarrow \boxed{f'(x) = \frac{1}{12\delta}[f(x-2\delta) - f(x+2\delta) + 8f(x+\delta) - 8f(x-\delta)] + \frac{\delta^4}{30} f^{V}(\xi)}$$

for some ξ s.t. $x - 2\delta < \xi < x + 2\delta$ by Taylor's Theorem

b. → $\frac{\delta^4}{30} f^{V}(\xi)$ is our truncation error (e_t) from the expansion
→ the machine also has round-off error

$e_r \sim \frac{\varepsilon f(x)}{\delta}$ where ε is the machine accuracy

→

1.6. → our total error estimate is

$$E \approx e_r + e_T \approx \frac{\varepsilon f(x)}{\delta} + \frac{\delta^4 f^{v}(\xi)}{30}$$

→ to minimize E,

$$0 = \frac{\partial E}{\partial \delta} \approx \frac{2}{15}\delta^3 f^{v}(\xi) - \frac{\varepsilon f(x)}{\delta^2}$$

$$\Rightarrow \delta^5 \approx \frac{15\varepsilon f(x)}{2 f^{v}(\xi)} \sim \varepsilon$$

$\Rightarrow \delta \approx \sqrt[5]{\varepsilon}$ very roughly minimizes error

$$\Rightarrow \boxed{\delta \approx \begin{cases} \sqrt[5]{10^{-16}} \approx 6.3 \times 10^{-4} & \text{for Double Precision} \\ \sqrt[5]{10^{-8}} \approx 2.5 \times 10^{-2} & \text{for Single Precision} \end{cases}}$$

→ my main concerns from this estimation come from my assumption

$e_r \approx \frac{\varepsilon f(x)}{\delta}$ as it was in class

and from my assumption

$$\frac{15 f(x)}{2 f^{v}(\xi)} \approx 1$$

→ I used both my class notes and Numerical Recipes section 5.7 to arrive at these rough estimates