PHYS 512: Assignment 1

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1. a) First we look at Taylor series for f at the four points $x \pm \delta$, $x \pm 2\delta$:

$$① \; f(x+\delta) = f(x) + \delta f'(x) + \tfrac{1}{2}\delta^2 f''(x) + \tfrac{1}{6}\delta^3 f'''(x) + O(\delta^4)$$
$$② \; f(x-\delta) = f(x) - \delta f'(x) + \tfrac{1}{2}\delta^2 f''(x) - \tfrac{1}{6}\delta^3 f'''(x) + O(\delta^4)$$
$$③ \; f(x+2\delta) = f(x) + 2\delta f'(x) + 2\delta^2 f''(x) + \tfrac{4}{3}\delta^3 f'''(x) + O(\delta^4)$$
$$④ \; f(x-2\delta) = f(x) - 2\delta f'(x) + 2\delta^2 f''(x) - \tfrac{4}{3}\delta^3 f'''(x) + O(\delta^4)$$

Subtracting ② from ①, we get

$$⑤ \; f(x+\delta) - f(x-\delta) = 2\delta f'(x) + \tfrac{1}{3}\delta^3 f'''(x) + O(\delta^5)$$ ← because even-power terms cancel

And subtracting ④ from ③ gives us

$$⑥ \; f(x+2\delta) - f(x-2\delta) = 4\delta f'(x) + \tfrac{8}{3}\delta^3 f'''(x) + O(\delta^5)$$

Now, to cancel the δ^3 term, we can subtract ⑥ from 8·⑤:

$$⑦ \; 8f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta) = 12\delta f'(x) + O(\delta^5)$$

So we can solve for $f'(x)$ to get our new rule:

$$\boxed{f'(x) = \frac{8f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta)}{12\delta}} + O(\delta^4)$$

b) Let us look at the fourth order terms in ①-④:

$$①: \tfrac{1}{5!}\delta^5 f^{(5)}(x) \qquad ②: -\tfrac{1}{5!}\delta^5 f^{(5)}(x)$$
$$③: \tfrac{1}{5!}(2\delta)^5 f^{(5)}(x) = \tfrac{32}{5!}\delta^5 f^{(5)}(x) \qquad ④: -\tfrac{32}{5!}\delta^5 f^{(5)}(x)$$

So the leading order error in ⑤ and ⑥ are:

$$⑤: \tfrac{2}{5!}\delta^5 f^{(5)}(x) = \tfrac{1}{60}\delta^5 f^{(5)}(x)$$
$$⑥: 64/120 \cdot \delta^5 f^{(5)}(x) = \tfrac{8}{15}\delta^5 f^{(5)}(x)$$

The leading order error in ⑦ would then be

$$\tfrac{8}{60}\delta^5 f^{(5)}(x) - \tfrac{8}{15}\delta^5 f^{(5)}(x) = -\tfrac{2}{5}\delta^5 f^{(5)}(x)$$

So the leading order error in our new rule for $f'(x)$ is

$$\left(\tfrac{2}{5}\delta^5 f^{(5)}(x)\right)/12\delta) = \tfrac{1}{30}\delta^4 f^{(5)}(x)$$

From class we had truncation error $\approx \epsilon f/\delta$, so

to minimize

we minimize the variance

$$\left(\frac{\varepsilon f}{\delta}\right)^2 + \left(\frac{1}{30}\delta^4 f^{(5)}(x)\right)^2 = \frac{\varepsilon^2 f^2}{\delta^2} + \left(\frac{f^{(5)}}{30}\right)^2 \delta^8$$

by taking the derivative w.r.t. δ and setting it to 0:

$$-\frac{\varepsilon^2 f^2}{\delta^3} + \left(\frac{f^{(5)}}{30}\right)^2 \cdot 8\delta^7 = 0$$

$$\Rightarrow \left(\frac{f^{(5)}}{30}\right)^2 \cdot 8\delta^{10} = \varepsilon^2 f^2$$

$$\Rightarrow \delta^{10} = \frac{1}{8}\left(\frac{15\varepsilon f}{f^{(5)}}\right)^2$$

Ignoring coefficients, we get

$$\delta \approx \sqrt[5]{\frac{\varepsilon f}{f^{(5)}}}$$

to be the ideal step size. We approximate $f/f^{(5)} \approx 1$ and use $\delta = \sqrt[5]{\varepsilon}$ in our code.