Phys 512 Pset 1

1. a) $f' = \dfrac{f(x+\delta)-f(x-\delta)}{2\delta}$, $f' = \dfrac{f(x+2\delta)-f(x-2\delta)}{4\delta}$

$$f(x\pm\delta) = f(x) \pm \delta f'(x)\, x + \delta \frac{f''(x)}{2} x^2 \pm \frac{f'''(x)}{6}\delta x^3 + \frac{f''''(x)}{24}\delta x^4 \pm \frac{f'''''(x)}{120}\delta x^5$$

$$f(x\pm 2\delta) = f(x) \pm 2f'(x)\delta x + 2f''(x)\delta x^2 \pm \frac{4}{3} f'''(x)\delta x^3 + \frac{2}{3} f''''(x)\delta x^4 \pm \frac{4}{15} f'''''(x)\delta x^5$$

Want to cancel the x^2 term: $a + b\delta x^2 + c\delta x^4$ (since odd power terms are already cancelled)

i.e. want:

$$a\left[\frac{f(x+2\delta)-f(x-2\delta)}{4\delta x}\right] + b\left[\frac{f(x+\delta)-f(x-\delta)}{2\delta x}\right] = f'(x)\delta x + \underbrace{c f'''''(x)\delta x^5}_{\text{want to cancel } x^3 \text{ term}}$$

$$\Rightarrow a\left[\frac{4f'(x)\delta x + \frac{8}{3}f'''(x)\delta x^3 + \frac{8}{15} f'''''(x)\delta x^5 + \cdots}{4\delta x}\right] + b\left[\frac{2f'(x)\delta x + \frac{1}{3} f'''(x)\delta x^3 + \frac{1}{60} f'''''(x)\delta x^5 + \cdots}{2\delta x}\right]$$

$$= a\left[f'(x) + \frac{2}{3} f'''(x)\delta x^2 + \frac{8}{60} f'''''(x)\delta x^4 + \cdots\right] + b\left[f'(x) + \frac{1}{6} f'''(x)\delta x^2 + \frac{1}{120} f'''''(x)\delta x^4 + \cdots\right]$$

Find a, b, c to cancel out $f'''(x)$ & $f'''''(x)$ term on RHS is satisfied:

$$\frac{2}{3}a = -\frac{1}{6}b$$

& RHS $\quad \frac{8}{60}a + \frac{1}{120}b = c \;\rightarrow\; a = -\frac{1}{3},\; b = \frac{4}{3}$

f' term gives: $a + b = c$

$$\Rightarrow -\frac{1}{3}f'(x) - \cancel{\frac{2}{9}f'''(x)\delta x^2} - \frac{2}{45} f'''''(x)\delta x^4 + \cdots + \frac{4}{3}f'(x) + \cancel{\frac{2}{9} f'''(x)\delta x^2} + \frac{1}{90} f'''''(x)\delta x^4 \cdots$$

$$= f'(x) - \frac{1}{30} f'''''(x)\delta x^4 + \cdots$$

$$\Rightarrow f'(x) = \underbrace{\frac{4(f(x+\delta)-f(x-\delta))}{6\delta x} - \frac{(f(x+2\delta)-\delta(x-2\delta))}{12\delta}}_{\text{numerical derivative}} + \underbrace{\frac{1}{30} f'''''(x)\,\delta^4}_{\text{error term (leading order)}}$$

b) Roundoff Error: $\underbrace{\bar{f}(x)}_{\text{bin. rep.}} = \underbrace{f(x)}_{\text{true val}} + \underbrace{\epsilon f(x)}_{\text{roundoff error}}$

$$\to \text{Error } \tilde{f} = f'(x) - \frac{4\left(\bar{f}(x+\delta) - \bar{f}(x-\delta)\right)}{6\delta} + \frac{\left(\bar{f}(x+2\delta) - \bar{f}(x-2\delta)\right)}{12\delta}$$

$$\tilde{f} = f'(x) - \frac{4\left(f(x+\delta) - f(x-\delta)\right)}{6\delta} + \frac{\left(f(x+2\delta) - f(x-2\delta)\right)}{12\delta}$$

$$+ \frac{4\epsilon\left(f(x+\delta) - f(x-\delta)\right)}{6\delta} - \frac{\epsilon\left(f(x+2\delta) - f(x-2\delta)\right)}{12\delta}$$

$$\tilde{f} = \frac{1}{30} f'''''(x)\,\delta^4 + \frac{18}{12\delta}\epsilon f(x)$$

Want to minimize: $\frac{\partial \tilde{f}}{\partial \delta} = \frac{1}{15} f'''''(x)\,\delta^3 - \frac{3\epsilon}{2\delta^2} f(x) = 0$

$$\to \delta^3 f'''''(x) = \frac{45}{2} \frac{\epsilon}{\delta^2} f(x)$$

$$\boxed{\delta^* = \left[\frac{45}{2}\epsilon \frac{f(x)}{f'''''(x)}\right]^{1/5}}$$

Optimal value of δ