Phys 512 HW1

1) (a) First, Taylor-expand $f(x \pm \delta)$ & $f(x \pm 2\delta)$:

$$
\begin{cases}
f(x+\delta) = f(x) + \delta f'(x) + \frac{1}{2!}\delta^2 f''(x) + \frac{1}{3!}\delta^3 f''' + \frac{1}{4!}\delta^4 f^{(4)} + \frac{1}{5!}\delta^5 f^{(5)} \\
f(x-\delta) = f - \delta f' + \frac{1}{2!}\delta^2 f'' - \frac{1}{3!}\delta^3 f''' + \frac{1}{4!}\delta^4 f^{(4)} - \frac{1}{5!}\delta^5 f^{(5)} \\
f(x+2\delta) = f + 2\delta f' + \frac{1}{2!}(2\delta)^2 f'' + \frac{1}{3!}(2\delta)^3 f''' + \frac{1}{4!}(2\delta)^4 f^{(4)} + \frac{1}{5}(2\delta)^5 f^{(5)} \\
f(x-2\delta) = f - 2\delta f' + \frac{1}{2!}(2\delta)^2 f'' - \frac{1}{3!}(2\delta)^3 f''' + \frac{1}{4!}(2\delta)^4 f^{(4)} - \frac{1}{5!}(2\delta)^5 f^{(5)}
\end{cases}
$$

→ Let's try $f(x+\delta) - f(x-\delta)$ as with the usual double-sided derivative:

$$f(x+\delta) - f(x-\delta) = 2\delta f' + 2\frac{1}{3!}\delta^3 f''' + \frac{1}{5!}\delta^5\left(f^{(5)}(\varepsilon_1) - f^{(5)}(\varepsilon_2)\right)$$

→ What if we now do $f(x+2\delta) - f(x-2\delta)$?

$$f(x+2\delta) - f(x-2\delta) = 4\delta f' + 2\frac{1}{3!}(2\delta)^3 f''' + \frac{1}{5!}\delta^5\left(f^{(5)}(\varepsilon_3) - f^{(5)}(\varepsilon_4)\right)$$

→ Now we can get rid of the f''' term as follows:

$$2^3\left(f(x+\delta) - f(x-\delta)\right) - \left(f(x+2\delta) - f(x-2\delta)\right)$$

$$= 12\delta f' + \frac{1}{5!}\delta^5\left(2^3\left(f^{(5)}(\varepsilon_1) - f^{(5)}(\varepsilon_2)\right) - \left(f^{(5)}(\varepsilon_3) - f^{(5)}(\varepsilon_4)\right)\right)$$

This leads to

$$\boxed{f'(x) \sim \frac{2^3\left(f(x+\delta) - f(x-\delta)\right) - \left(f(x+2\delta) - f(x-2\delta)\right)}{12\delta}}$$

With error on the order of δ^4.

(b) If we assume a roundoff error $e_r \sim \frac{\epsilon_f f}{\delta}$, and we see that $e_t \sim \delta^5 f^{(5)}$, we can optimize δ as follows:

$$e_{tot} = e_r + e_t \sim \frac{\epsilon_f f}{\delta} + \delta^5 f^{(5)}$$

$$\frac{de_{tot}}{d\delta} \sim -\frac{\epsilon_f f}{\delta^2} + 5\delta^4 f^{(5)} = 0 \leftarrow \text{minimize}$$

$$\frac{\epsilon_f f}{\delta^2} \sim 5\delta^4 f^{(5)}$$

$$\delta^6 \sim \frac{\epsilon_f f}{5 f^{(5)}}$$

$$\delta \sim \left(\frac{\epsilon_f f}{5 f^{(5)}}\right)^{1/6}$$

And we can (safely?) approximate

$$\boxed{\delta \sim (\epsilon_f)^{1/6}}$$

as our optimal δ, where ϵ_f is the fractional accuracy.