PHYS 512: Problem Set 1

Problem 1:

a) Using the Taylor series expansion, we have:

$$f(x+2\delta) = f(x) + 2\delta f'(x) + 4\delta^2 \frac{f''(x)}{2} + 8\delta^3 \frac{f'''(x)}{6} + 16\delta^4 \frac{f^{(4)}(x)}{24} + 32\delta^5 \frac{f^{(5)}(x)}{120}$$

$$f(x-2\delta) = f(x) - 2\delta f'(x) + 4\delta^2 \frac{f''(x)}{2} - 8\delta^3 \frac{f'''(x)}{6} + 16\delta^4 \frac{f^{(4)}(x)}{24} - 32\delta^5 \frac{f^{(5)}(x)}{120}$$

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

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

Then: $f(x+2\delta) - f(x-2\delta) = 4\delta f'(x) + 16\delta^3 \frac{f'''(x)}{6} + 64\delta^5 \frac{f^{(5)}(x)}{120}$

$$f(x+\delta) - f(x-\delta) = 2\delta f'(x) + 2\delta^3 \frac{f'''(x)}{6} + 2\delta^5 \frac{f^{(5)}(x)}{120}$$

Since we want to eliminate f''' term and keep the f', we can do:

$$f(x+2\delta) - f(x-2\delta) - 8(f(x+\delta) - f(x-\delta)) = -12\delta f'(x) + 48\delta^5 \frac{f^{(5)}(x)}{120}$$

and $f'(x) = \dfrac{8f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta)}{12\delta} + \delta^4 \dfrac{f^{(5)}(x)}{30}$

where $\dfrac{\delta^4 f^{(5)}(x)}{30} = e_t$ is the truncation error.

b) We know that the total error is $e_r + e_t$ where e_r is the roundoff error, equal to:

$$e_r = \varepsilon_f \left| \frac{f(x)}{\delta} \right| \quad , \varepsilon_f \approx \text{machine epsilon}$$

So $e_r + e_t \approx \varepsilon \frac{f(x)}{\delta} + \delta^4 f^{(5)}(x)$. In order to find the optimal δ we differentiate with respect to δ and find the value that sets our derivative to 0:

$$\frac{d(e_r+e_t)}{d\delta} \sim \delta^3 f^{(5)}(x) - \varepsilon \frac{f(x)}{\delta^2} = 0 \iff \underline{\delta \sim \left(\frac{\varepsilon f(x)}{f^{(5)}(x)}\right)^{1/5}}$$