PHYS - 512 PS1

#1

a)

$$f(x+\delta) = f(x) + \delta f'(x) + \frac{\delta^2}{2!} f''(x) + \frac{\delta^3}{3!} f'''(x) + O(\delta^4)$$

$$f(x-\delta) = f(x) - \delta f'(x) + \frac{\delta^2}{2!} f''(x) - \frac{\delta^3}{3!} f'''(x) + O(\delta^4)$$

$$f(x+2\delta) = f(x) + 2\delta f'(x) + \frac{(2\delta)^2}{2!} f''(x) + \frac{(2\delta)^3}{3!} f'''(x) + O(\delta^4)$$

$$f(x-2\delta) = f(x) - 2\delta f'(x) + \frac{(2\delta)^2}{2!} f''(x) - \frac{(2\delta)^3}{3!} f'''(x) + O(\delta^4)$$

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

② $$f'(x) = \frac{f(x+2\delta) - f(x-2\delta)}{4\delta} = \frac{4\delta f'(x) + \frac{16\delta^3}{3!} f'''(x)}{4\delta}$$

To cancel out the error term:

$$4 \times ① - ② = \frac{16\delta f'(x) + \cancel{\frac{16\delta^3}{3!} f'''(x)} - 4\delta f'(x) - \cancel{\frac{16\delta^3}{3!} f'''(x)}}{4\delta}$$

$$4\left[\frac{f(x+\delta) - f(x-\delta)}{2\delta}\right] - \left[\frac{f(x+2\delta) - f(x-2\delta)}{4\delta}\right] = 3f'(x)$$

$$f'(x) = \frac{2f(x+\delta) - 2f(x-\delta)}{3\delta} - \frac{f(x+2\delta) - f(x-2\delta)}{12\delta}$$

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

b) Since the roundoff error of the two-sided derivation is $e_r \sim \frac{\varepsilon f}{dx}$, and the truncation error is $e_t \sim dx^2 f'''$,

$$\text{Total error} = \frac{\varepsilon f}{dx} + dx^2 f'''$$

To minimize it,

$$\frac{d}{dx}\left(\frac{\varepsilon f}{dx} + dx^2 f'''\right) = \frac{-\varepsilon f}{dx^2} + 2\,dx\,f'''$$

$$0 = -\frac{\varepsilon f}{dx^2} + 2\,dx\,f'''$$

$$dx\,f''' = \frac{\varepsilon f}{dx^2}$$

$$dx = \left(\frac{\varepsilon f}{f'''}\right)^{1/3}$$

For $f(x) = \exp(x)$, $\frac{f}{f'''} = 1 \Rightarrow dx = \varepsilon^{1/3}$

For $f(x) = \exp(0.01x)$, $\frac{f}{f'''} = 10^4 \Rightarrow dx = \varepsilon^{1/3} \cdot 10^{4/3}$

#4

The error is larger for the Lorentzian.
After using np.linalg.pinv, the error decreased significantly from 0.8186 to 1.549 e-16.