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PHYS 512 _ Assignment 1 .

(*) Problem 1 :

a) . $f(x \pm \delta) \simeq f(x) \pm f'(x)\delta + \frac{1}{2} f''(x).\delta^2 \pm \frac{1}{6} f'''(x).\delta^3 + \ldots$

$\Rightarrow f(x+\delta) - f(x-\delta) = 2f'(x)\delta + \frac{1}{3} f'''(x).\delta^3 + \ldots$ (1)

. $f(x \pm 2\delta) \simeq f(x) \pm 2.f'(x)\delta + 4.\frac{1}{2} f''(x).\delta^2 \pm 8.\frac{1}{6} f'''(x)\delta^3 + \ldots$

$\Rightarrow f(x+2\delta) - f(x-2\delta) = 4f'(x)\delta + \frac{8}{3} f'''(x).\delta^3 + \ldots$ (2)

(1) & (2) :

$8[f(x+\delta) - f(x-\delta)] - [f(x+2\delta) - f(x-2\delta)] = 12 f'(x).\delta$

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

b) We will modify $f(x) \to (1 + g_i \varepsilon) f(x)$ to take into account machine precision . $\varepsilon \sim 10^{-6}$ is the machine error whereas g_i is the order unity random number.

The derivative of the modified function is $\tilde{f}'(x)$ and by the same procedure as before can be found to be :

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

Error from our previous calculation :

$$\text{Error} = f'(x) - \tilde{f}'(x)$$

$$\Leftrightarrow \quad \text{Error} = \cancel{f'(x)} - \cancel{\frac{8[f(x+\delta) - f(x-\delta)] - [f(x+2\delta) - f(x-2\delta)]}{12\delta}}$$

$$- \varepsilon \cdot \frac{8[g_1\tilde{f}(x+\delta) - g_2\tilde{f}(x-\delta)] - [g_3\tilde{f}(x+2\delta) - g_4\tilde{f}(x-2\delta)]}{12\delta} \qquad (3)$$

Note that there are still some error terms in the expression of $f'(x)$ above that we might have ignored. Redo the math and we have:

$$f'(x) = \cancel{\frac{8[f(x+\delta) - f(x-\delta)] - [f(x+2\delta) - f(x-2\delta)]}{12\delta}} + \frac{f^5}{30}\delta^4 \qquad (4)$$

(3) & (4):

$$\text{Error} = \frac{f^{(5)}}{30}\delta^4$$

$$- \varepsilon \cdot \frac{8[g_1\tilde{f}(x+\delta) - g_2\tilde{f}(x-\delta)] - [g_3\tilde{f}(x+2\delta) - g_4\tilde{f}(x-2\delta)]}{12\delta}$$

For maximum error, we'll choose $-g_1 = +g_2 = +g_3 = -g_4 = 1$.

$$\Rightarrow \quad \text{Error} \leq \frac{f^{(5)}\delta^4}{30} + \varepsilon \frac{18}{12}\frac{f(x)}{\delta} = \frac{f^{(5)}\delta^4}{30} + \frac{3}{2}\varepsilon\frac{f}{\delta}$$

Error is minimized when: $\frac{d\,\text{Error}}{d\delta} = 0 \quad \Leftrightarrow \quad \frac{2}{15} f^{(5)}\delta^3 - \frac{3}{2}\varepsilon\frac{f}{\delta^2} = 0$

$$\Rightarrow \quad \delta = \sqrt[5]{\frac{45}{4}\varepsilon\frac{f(x)}{f^{(5)}(x)}}$$

⊛ Problem 3:

$$y = \frac{1}{1+x^2} = \frac{P(x)}{Q(x)} = \frac{p_0 + p_1x + p_2x^2 + \dots}{1 + q_1x + q_2x^2 + \dots}$$

$$\Leftrightarrow \quad y \cdot Q(x) = P(x)$$

$$\Leftrightarrow \quad y + q_1yx + q_2yx^2 + q_3yx^3 = p_0 + p_1x + p_2x^2 + p_3x^3 + \dots$$

$$\Leftrightarrow \quad y = p_0 + p_1x + p_2x^2 + \dots + p_{m-1}x^{m-1} + p_mx^m +$$

$$- q_1 y x - q_2 y x^2 - \dots - q_{n-1} x^{n-1} - q_n x^n$$

- If we stop at order $m-1$ & $n-1$, then the maximized error is:

$$\text{Error} \lesssim p_m x^m + q_n x^n$$

- For the Lorentzian, p_m & q_n are relatively small for high order m & n and relatively large for small order m & n.

  $\Rightarrow$ The error on the rational fit will be very low for high order m & n

  $\Rightarrow$ This agrees with what we see in the code.