Problem Set I (18/09/20)

Q.1] For function f, given at following points

$x-2\delta \quad x-\delta \quad x \quad x+\delta \quad x+2\delta$

a) Writing out the Taylor exp. at each point

$$f(x+\delta) = f(x) + \delta . f'(x) + \frac{\delta^2}{2} f''(x) + \frac{\delta^3}{6} f'''(x) + \frac{\delta^4}{24} f''''(x)$$
$$+ \frac{\delta^5}{120} f'''''(x) + \ldots + g_1 \xi \qquad \{ \xi \leftarrow \text{round off error} \}$$

Similarly,

$$f(x-\delta) = f(x) - \delta f'(x) + \frac{\delta^2}{2} f''(x) - \frac{\delta^3}{6} f'''(x) + \frac{\delta^4}{24} f''''(x) - \frac{\delta^5}{120} f'''''(x) + \ldots g_2 \xi$$

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

$$f(x-2\delta) = f(x) - 2\delta f'(x) + 2\delta^2 f''(x) - \frac{4\delta^3}{3} f'''(x) + \frac{2\delta^4}{3} f''''(x) - \frac{4\delta^5}{15} f'''''(x) + \ldots g\xi$$

The most basic definition for derivative of f at x.

$$f'(x) = \frac{f(x+\delta) - f(x)}{\delta} = \underbrace{\left(\frac{\delta}{2} f''(x) + \frac{\delta^2}{6} f'''(x) + \ldots \right)}_{\text{Error}} + f'(x)$$

Leading error terms are from 2^{nd}, 3^{rd}... order terms.

- Using the $\pm\delta$ points, the even order terms can be easily cancelled, ie

$$\frac{f(x+\delta) - f(x-\delta)}{2\delta} = f'(x) + \frac{\delta^2}{6} f'''(x) + \frac{\delta^4}{120} f'''''(x) + \ldots \quad (1)$$

- Following this, we can utilsize the $\pm 2\delta$ terms to cancell the first odd order

$$\frac{f(x+2\delta) - f(x-2\delta)}{4\delta} = f'(x) + \frac{2}{3}\delta^2 f'''(x) + \frac{2\delta^4}{15} f'''''(x) + \ldots \quad (2)$$

Combining ① & ② such that the first odd term goes away

i.e. $\dfrac{(4 \times ①) - (②)}{3}$

$$\Rightarrow \frac{4}{3}\left[\frac{f(x+\delta)-f(x-\delta)}{2\delta}\right] - \frac{1}{3}\left[\frac{f(x+2\delta)-f(x-2\delta)}{4\delta}\right]$$

$$= \frac{1}{3}\Big[4f'(x) + \cancel{\frac{2}{3}\delta^2 f'''(x)} + \frac{\delta^4}{30} f'''''(x) + \ldots + g\xi/2\delta$$

$$- f'(x) - \cancel{\frac{2}{3}\delta^2 f'''(x)} - \frac{2}{15}\delta^4 f'''''(x) + \ldots + g\xi/4\delta\Big]$$

$$= f'(x) + \frac{1}{3}\left(\frac{1}{30} - \frac{4}{30}\right)\delta^4 . f'''''(x) + g_*\xi/\delta$$

$$= f'(x) - \frac{\delta^4}{30} f'''''(x) + g_*\xi/\delta$$

Hence defining $f'(x)$ as follows cancels 3 additional terms

$$f'(x) = \frac{1}{12\delta}\left(8f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta)\right)$$

Leading error term $\sim \delta^4 f'''''(x)$

- For optimal value of δ, we need to minimize the error i.e. for $E = \dfrac{\delta^4}{30} f'''''(x) + g_*\xi/\delta$

$$\frac{dE}{d\delta} = 0 \Rightarrow \frac{4\delta^3}{30} . f'''''(x) - \frac{g_* . \xi}{\delta^2} = 0$$

$$\Rightarrow \delta^5 = \frac{30 . g_* . \xi}{f'''''(x)}$$

$$\Rightarrow \delta \simeq \left(\frac{\xi}{f^{(5)}(x)}\right)^{1/5} \qquad \{ f''''' = f^{(5)} \}$$

b) For $f(x) = \exp(ax)$, $f^{(5)}(x) = a^5 . \exp(ax)$

$$\Rightarrow \text{Optimal, } \delta_{opt} = \left(\frac{\xi}{a^5 . \exp(ax)} \right)^{1/5}$$

$$= \frac{\xi^{1/5}}{a . \exp(ax/5)} \qquad \{ \xi = \text{machine precision} \}$$

As already discussed in class $\xi \simeq 10^{-16}$ or $\xi^{1/5} = 10^{-3.2}$

$\Rightarrow \xi^{1/5} \simeq 10^{-3}$ (appx).

For $a = 1$, $\delta_{opt} = \dfrac{10^{-3}}{1 . \exp(x)}$

$a = 0.01$, $\delta_{opt} = \dfrac{10^{-3}}{0.01 . \exp(0.01x)} = \dfrac{10^{-1}}{\exp(0.01x)}$