Problem 1

(a) The function evaluated in the four points is Taylor expanded as follows:

$$\rightarrow f(x+\delta) \approx f(x) + f'(x)\delta + \frac{1}{2} f''(x)\delta^2 + \frac{1}{6} f'''(x)\delta^3 + \dots \quad (1)$$

$$\rightarrow f(x-\delta) \approx f(x) - f'(x)\delta + \frac{1}{2} f''(x)\delta^2 - \frac{1}{6} f'''(x)\delta^3 + \dots \quad (2)$$

$$\rightarrow f(x+2\delta) = f(x) + 2f'(x)\delta + 2f''(x)\delta^2 + \frac{4}{3} f'''(x)\delta^3 + \dots \quad (3)$$

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

The idea is to find $f'(x)$ combining (1), (2), (3) and (4) in such a way that $f'(x)$ depends on the function $f(x)$ evaluated in the 4 points. That means, $f'(x)$ depends only of known variables.

- First (1) - (2):

$$\Rightarrow f(x+\delta) - f(x-\delta) = 2f'(x)\delta + \frac{1}{3} f'''(x)\delta^3 \quad (5)$$

- Then (3) - (4):

$$\Rightarrow f(x+2\delta) - f(x-2\delta) = 4f'(x)\delta + \frac{8}{3} f'''(x)\delta^3 \quad (6)$$

- Now (6) - 8·(5):

$$\Rightarrow f(x+2\delta) - f(x-2\delta) - 8\left[f(x+\delta) - f(x-\delta)\right] = 4f'(x)\delta + \cancel{\frac{8}{3} f'''(x)\delta^3} - 16f'(x)\delta \cancel{- \frac{8}{3} f'''(x)\delta^3}$$

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$$\Rightarrow f(x+2\delta) - f(x-2\delta) - 8\left[f(x+\delta) - f(x-\delta)\right] = -12 f'(x)\,\delta$$

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

(b) The total numerical error is the sum of the roundoff and truncation error.

Here, the idea is to find the step size δ that minimizes the total error.

$$\text{total error} = \underbrace{\text{truncation error}}_{f'(x)} + \underbrace{\text{roundoff error}}_{f'(x)}$$

I will work with each of them separately.

Truncation error

- comes from the Taylor expansion of each term in the derivative :

$$f'(x) = \frac{\overbrace{f(x-2\delta) - f(x+2\delta)}^{\mathrm{I}} + \overbrace{8f(x+\delta) - 8f(x-\delta)}^{\mathrm{II}}}{12\delta}$$

so I will Taylor expand each term I and II .

Term I

$\rightarrow f(x+2\delta) \approx f(x) + 2f'(x)\delta + 2f''(x)\delta^2 + \frac{4}{3}f'''(x)\delta^3 + f''''(x)\delta^4 \cdot \frac{16}{24} + f'''''(x)\delta^5 \cdot \frac{32}{120}$

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

$\rightarrow f(x-2\delta) - f(x+2\delta) \approx -4f'(x)\delta - \frac{8}{3}f'''(x)\delta^3 - 2f'''''(x)\delta^5 \cdot \frac{32}{120}$

$$= -4f'(x)\delta - \frac{8}{3}f'''(x)\delta^3 - \frac{4}{15}f'''''(x)\delta^5$$

$\rightarrow \frac{1}{12\delta}\left[f(x-2\delta) - f(x+2\delta)\right] = -\frac{4}{12\delta}f'(x)\delta - \frac{8}{12\delta \cdot 3}f'''(x)\delta^3 - \frac{4}{12\delta \cdot 15}f'''''(x)\delta^5$

$$\Rightarrow \boxed{\frac{1}{12\delta}\left[f(x-2\delta) - f(x+2\delta)\right] = -\frac{1}{3}f'(x) - \frac{2}{9}f'''(x)\delta^2 - \frac{1}{45}\delta^4 f'''''(x)}$$

Term II

$$\rightarrow f(x+\delta) \simeq f(x)+f'(x)\delta+\frac{1}{2}f''(x)\delta^2+\frac{1}{6}f'''(x)\delta^3+\frac{1}{24}f''''(x)\delta^4+\frac{1}{120}f'''''(x)\delta^5$$

$$\rightarrow f(x-\delta) \simeq f(x)-f'(x)\delta+\frac{1}{2}f''(x)\delta^2-\frac{1}{6}f'''(x)\delta^3+\frac{1}{24}f''''(x)\delta^4-\frac{1}{120}f'''''(x)\delta^5$$

$$\rightarrow f(x+\delta)-f(x-\delta) = 2f'(x)\delta+\frac{1}{3}f'''(x)\delta^3+\frac{1}{120}f'''''(x)\delta^5$$

$$\rightarrow \frac{8}{12\delta}\left[f(x+\delta)-f(x-\delta)\right] = \frac{8\cdot 2}{12\delta}f'(x)\delta+\frac{8}{12\delta\cdot 3}f'''(x)\delta^2+\frac{8}{12\delta\cdot 60}f'''''(x)\delta^5$$

$$\Rightarrow \boxed{\frac{8}{12\delta}\left[f(x+\delta)-f(x-\delta)\right] = \frac{4}{3}f'(x)+\frac{2}{9}f'''(x)\delta^2+\frac{1}{90}f'''''(x)\delta^4}$$

The sum of I and II is: $f'(x)-\frac{1}{45}f'''''(x)\delta^4$

so:

$$\boxed{\text{Truncation error} = -\frac{1}{45}f'''''(x)\delta^4} = \overline{f'(x)}$$

Randoff error

Comes from the machine precision. The randoff error will be given by:

$$\overline{\overline{f'(x)}} = f'(x)\left(1 + \varepsilon g\right)$$

where ε is the machine epsilon and g is a factor of order unity, let's say $g \in [-1, 1]$.

So:

$$\rightarrow \overline{\overline{f'(x)}} = \frac{f(x-2\delta)(1+\varepsilon g_{2-}) - f(x+2\delta)(1+\varepsilon g_{2+})}{12\delta}$$

$$+ \frac{8}{12\delta}\left[f(x+\delta)(1+\varepsilon g_{+}) - f(x-\delta)(1+\varepsilon g_{-})\right]$$

will quantify the randoff error. However, $f(x \pm 2\delta)$ and $f(x \pm \delta)$ must be Taylor expanded.

Since I'm trying to account for the maximum possible error, I will only consider the first term of the Taylor expansion. The error for the remainder terms is too small, and do not contribute to the randoff error as much as the first term.

$$\rightarrow f(x \pm \delta) \approx f(x)$$

$$\rightarrow f(x \pm 2\delta) \approx f(x)$$

then:

$$\rightarrow \overline{\overline{f'(x)}} = \frac{1}{12\delta}\left[\cancel{f(x)} + \varepsilon g_{2-} f(x) - \cancel{f(x)} - \varepsilon g_{2+}(x)\right]$$

$$+ \frac{8}{12\delta}\left[\cancel{f(x)} + \varepsilon g_{+} f(x) - \cancel{f(x)} - \varepsilon g_{-} f(x)\right]$$

Since g is a factor of order unity, it is convenient to choose

$g_{+} \to -1$ $\qquad$ $g_{-} \to +1$

$g_{2+} \to +1$ $\qquad$ $g_{2-} \to -1$

This also accounts for the biggest possible value of ε.

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

$$= \frac{-2}{12\delta}\varepsilon f(x) - \frac{8}{12\delta} \cdot 2\varepsilon f(x)$$

$$= -\frac{3}{2}\frac{\varepsilon f(x)}{\delta}$$

so:

$$\boxed{\text{Roundoff error} = -\frac{3}{2}\frac{\varepsilon f(x)}{\delta}} = \overline{\overline{f'(x)}}$$

Since the idea is to choose the step size δ that minimizes the total error:

$$\frac{d}{d\delta}\left(\underbrace{\frac{-3\varepsilon f(x)}{2\delta}}_{f'(x)} - \underbrace{\frac{1}{45} f'''''(x)\,\delta^4}_{f'(x)}\right) = 0$$

$$\rightarrow \; -\frac{3\varepsilon f(x)}{2}\cdot\left(-\frac{1}{\delta^2}\right) - \frac{4}{45} f'''''(x)\,\delta^3 = 0$$

$$\rightarrow \; \frac{3\varepsilon f(x)}{2\delta^2} = \frac{4}{45} f'''''(x)\,\delta^3$$

$$\rightarrow \; \delta^5 = \frac{3}{2}\varepsilon f(x)\cdot\frac{45}{4}\cdot\frac{1}{f'''''(x)}$$

So the optimal δ is:

$$\delta \sim \left(\frac{\varepsilon f(x)}{f'''''(x)}\right)^{1/5}$$

Because $\varepsilon \sim 10^{-16}$ for double precision:

$$\boxed{\delta \sim 10^{-16/5}}$$