PHYS 512
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Assignment 1

1

Evaluate our function f @ $(x \pm \delta)$ & $(x \pm 2\delta)$

a) What should our estimate of the first derivative at x be?

Use Taylor series expansion @ $(x \pm \delta)$ & $(x \pm 2\delta)$:

$$f(x \pm \delta) = f(x) \pm f^{(1)}(x)\delta + \frac{1}{2} f^{(2)}(x)\delta^2 \pm \frac{1}{6} f^{(3)}(x)\delta^3 + \frac{1}{24} f^{(4)}(x)\delta^4 \pm \frac{1}{120} f^{(5)}(x)\delta^5 + \mathcal{O}(\delta^6)$$

$$f(x \pm 2\delta) = f(x) \pm 2f^{(1)}(x)\delta + 4f^{(2)}(x)\delta^2 \pm \frac{4}{3} f^{(3)}(x)\delta^3 + \frac{2}{3} f^{(4)}(x)\delta^4 \pm \frac{4}{15} f^{(5)}(x)\delta^5 + \mathcal{O}(\delta^6)$$

From numerical recipes § 5.7 p. 230, we have a symmetrized form

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

For $h = \delta$: $$f_1'(x) \approx \frac{f(x+\delta) - f(x-\delta)}{2\delta} \quad (1)$$

for $h = 2\delta$: $$f_2'(x) \approx \frac{f(x+2\delta) - f(x-2\delta)}{4\delta} \quad (2)$$

① : $2\delta f_1^{(1)}(x) \approx f(x+\delta) - f(x-\delta)$

$$= \cancel{f(x)} + f^{(1)}(x)\delta + \cancel{\tfrac{1}{2}f^{(2)}(x)\delta^2} + \tfrac{1}{6}f^{(3)}(x)\delta^3 + \cancel{\tfrac{1}{24}f^{(4)}(x)\delta^4} + \tfrac{1}{120}f^{(5)}(x)\delta^5$$

$$- \left(\cancel{f(x)} - f^{(1)}(x)\delta + \cancel{\tfrac{1}{2}f^{(2)}(x)\delta^2} - \tfrac{1}{6}f^{(3)}(x)\delta^3 + \cancel{\tfrac{1}{24}f^{(4)}(x)\delta^4} - \tfrac{1}{120}f^{(5)}(x)\delta^5\right)$$

$$= 2f^{(1)}(x)\delta + \tfrac{1}{3}f^{(3)}(x)\delta^3 + \tfrac{1}{60}f^{(5)}(x)\delta^5$$

$$\Rightarrow 2\delta f_1^{(1)}(x) \approx 2f^{(1)}(x)\delta + \tfrac{1}{3}f^{(3)}(x)\delta^3 + \tfrac{1}{60}f^{(5)}(x)\delta^5 \qquad ③$$

② : $4\delta f_1^{(1)}(x) \approx f(x+2\delta) - f(x-2\delta)$

Much like with $h=\delta$, here the even n^{th}-derivative terms cancel out; the odd n^{th}-derivative terms are doubled

$$\Rightarrow 4\delta f_2^{(1)}(x) \approx 4f^{(1)}(x)\delta + \tfrac{8}{3}f^{(3)}(x)\delta^3 + \tfrac{8}{15}f^{(5)}(x)\delta^5 \qquad ④$$

How to combine ③ & ④ to cancel δ^3 terms?
From their coefficients, take:

$$8(③) - (④) \Rightarrow 8\left(2\delta f_1^{(1)}(x)\right) - \left(4\delta f_2^{(1)}(x)\right)$$

$$=$$

$$8\left(2f^{(1)}(x)\delta + \tfrac{1}{60}f^{(5)}(x)\delta^5\right)$$

$$-\left(4f^{(1)}(x)\delta + \tfrac{8}{15}f^{(5)}(x)\delta^5\right)$$

$$\Rightarrow 16\delta f_1^{(1)}(x) - 4\delta f_2^{(1)}(x)$$

$$=$$

$$16f^{(1)}(x)\delta + \tfrac{2}{15}f^{(5)}(x)\delta^5 - 4f^{(1)}(x)\delta - \tfrac{8}{15}f^{(5)}(x)\delta^5$$

$$\Rightarrow 16\delta f_1^{(1)}(x) - 4\delta f_2^{(1)}(x) = 12f^{(1)}(x)\delta - \tfrac{2}{5}f^{(5)}(x)\delta^5$$

$\Rightarrow$ We can isolate $f^{(1)}(x)$:

$$12 f^{(1)}(x)\,\delta = 16\delta f_1^{(1)}(x) - 4\delta f_2^{(1)}(x) + \frac{2}{5} f^{(5)}(x)\,\delta^5$$

$$\Rightarrow f^{(1)}(x) = \frac{1}{12\delta}\left[16\delta f_1^{(1)}(x) - 4\delta f_2^{(1)}(x) + \frac{2}{5} f^{(5)}(x)\,\delta^5\right]$$

$$= \frac{1}{12\delta}\left(16\delta\left[\frac{f(x+\delta)-f(x-\delta)}{2\delta}\right] - 4\delta\left[\frac{f(x+2\delta)-f(x-2\delta)}{4\delta}\right]\right) + \frac{1}{30} f^{(5)}(x)\,\delta^4$$

$$f^{(1)}(x) = \frac{1}{12\delta}\Big(8\big(f(x+\delta)-f(x-\delta)\big) - \big(f(x+2\delta)-f(x-2\delta)\big)\Big) + \frac{1}{30} f^{(5)}(x)\,\delta^4$$

We hence have an estimate of $f^{(1)}(x)$:

$$\boxed{f^{(1)}(x) = \frac{1}{12\delta}\Big[8\big(f(x+\delta)-f(x-\delta)\big) - \big(f(x+2\delta)-f(x-2\delta)\big)\Big] + \frac{1}{30} f^{(5)}(x)\,\delta^4 + \mathcal{O}(\delta^5)}$$