PHYS 512 Problem set 1

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Given a function f, evaluated at the points $x \pm \delta$ and $x \pm 2\delta$.

1.1 a)

The derivative at x can be calculated from the points around x using the central derivative formula (in the limit of small δ):

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

Performing a Taylor expansion of f at each point gives

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

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

$$f(x+2\delta) \approx f(x) + f'(x)2\delta + 2f''(x)\delta^2 + \frac{4}{3}f'''(x)\delta^3 + \frac{2}{3}f''''(x)\delta^4 + \frac{4}{15}f'''''(x)\delta^5 + ...$$

$$f(x-2\delta) \approx f(x) - f'(x)2\delta + 2f''(x)\delta^2 - \frac{4}{3}f'''(x)\delta^3 + \frac{2}{3}f''''(x)\delta^4 - \frac{4}{15}f'''''(x)\delta^5 + ...$$

For the $x \pm \delta$ case, subtracting $f(x-\delta)$ from $f(x+\delta)$ gives the central derivative:

$$f(x+\delta) - f(x-\delta) = 2f'(x)\delta + \frac{1}{3}f'''(x)\delta^3 + \frac{1}{60}f'''''(x)\delta^5 + ...$$

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

Performing the same operation on the $x \pm 2\delta$ case:

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

The δ^2 term can be eliminated by subtracting four times the $x \pm \delta$ derivative from the $x \pm 2\delta$ derivative

$$f'(x) - 4f'(x) = \left(\frac{f(x+2\delta) - f(x-2\delta)}{4\delta} - \frac{2}{3}f'''(x)\delta^2 - \frac{2}{15}f'''''(x)\delta^4 - ...\right) - 4\left(\frac{f(x+\delta) - f(x-\delta)}{2\delta} - \frac{1}{6}f'''(x)\delta^2 - \frac{1}{120}f'''''(x)\delta^4 + ...\right)$$

$$-3f'(x) = \frac{8f(x-\delta) + f(x+2\delta) - 8f(x+\delta) - f(x-\delta)}{4\delta} - \frac{1}{10}f'''''(x)\delta^4$$

$$\boxed{f'(x) = \frac{8f(x+\delta) - 8f(x-\delta) + f(x-\delta) - f(x+2\delta)}{12\delta} + \frac{1}{30}f'''''(x)\delta^4 + ...}$$

1.2 b)

The error for this derivative is comes from rounding error and discarding higher order terms from the Taylor series. For rounding error ϵ, the error is approximately

$$\text{error } = \frac{|f(x)| \cdot \epsilon}{\delta} + \frac{1}{30} f'''''(x)\delta^4.$$

Minimizing with respect to δ:

$$0 = \frac{\mathrm{d}}{\mathrm{d}\delta}\left(\frac{|f(x)| \cdot \epsilon}{\delta} + \frac{1}{30} f'''''(x)\delta^4\right) = -\frac{|f(x)| \cdot \epsilon}{\delta^2} + \frac{2}{15} f'''''(x)\delta^3$$

$$\frac{|f(x)| \cdot \epsilon}{\delta^2} = \frac{2}{15} f'''''(x)\delta^3$$

$$\delta^5 = \frac{15}{2}\frac{|f(x)| \cdot \epsilon}{f'''''(x)}$$

So the ideal value of δ should be

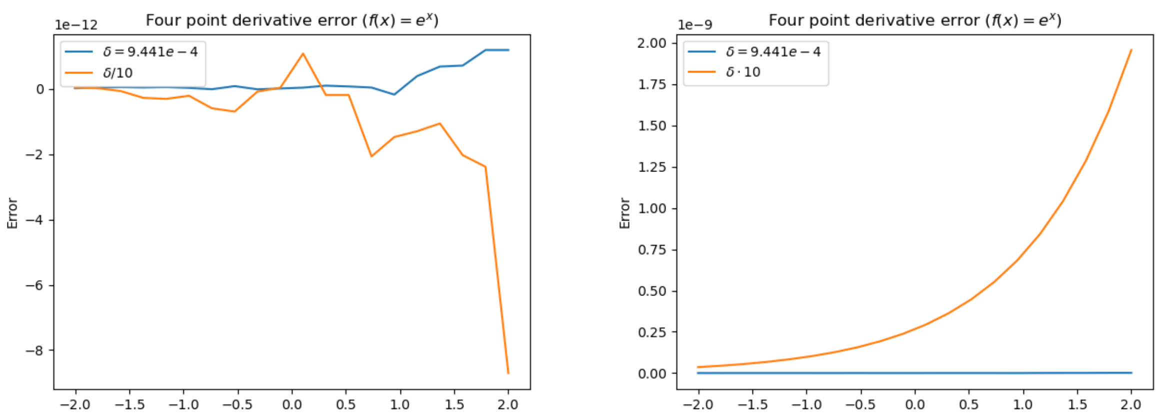
$$\boxed{\delta = \left(\frac{15}{2}\frac{|f(x)| \cdot \epsilon}{f'''''(x)}\right)^{1/5}}.$$

For $f = e^x$, the ideal step should be approximately

$$\delta \approx \left(\frac{15}{2}\frac{e^x}{e^x} \cdot 10^{-16}\right)^{1/5} = \left(\frac{15}{2} \cdot 10^{-16}\right)^{1/5} = 9.441 \cdot 10^{-4}$$

As shown in figure 1, the calculated value of δ performs better than steps sizes of an order of magnitude higher and lower.

Figure 1: Step size error comparison $f(x) = e^x$

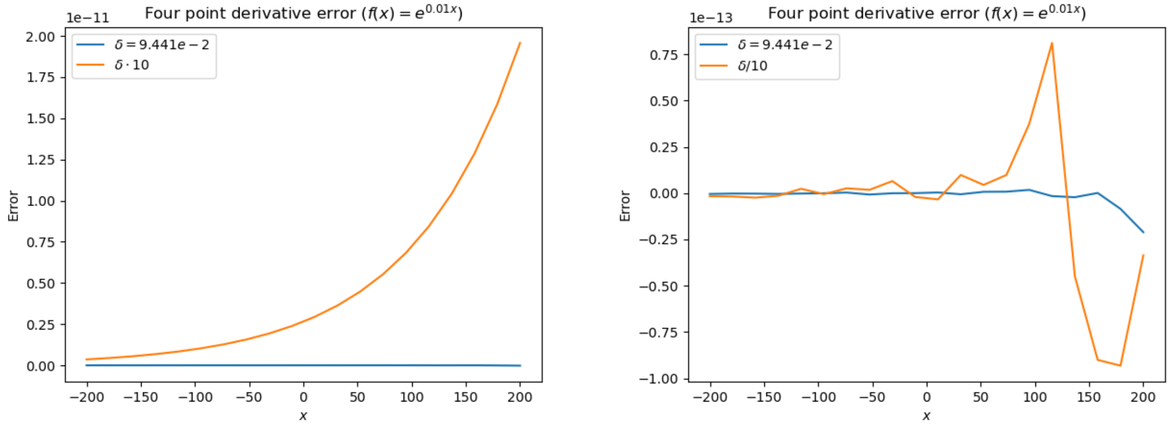


For $f(x) = e^{0.01x}$, the ideal step size should be approximately

$$\delta \approx \left(\frac{15}{2}\frac{e^{0.01x}}{10^{-10}e^{0.01x}} \cdot 10^{-16}\right)^{1/5} = \left(\frac{15}{2} \cdot 10^{-6}\right)^{1/5} = 9.441 \cdot 10^{-2}$$

As shown in Figure 2, this is also approximately the correct step size as it outperforms steps sizes of an order of magnitude larger and smaller.

Figure 2: Step size error comparison $f(x) = e^{0.01x}$



2

My numerical differentiator function pseudocode:
Finding optimal step size dx:

- To get around the proper order of magnitude, evaluate the derivative for $dx \in \{10^{-16}, 10^{-15}, 10^{-14}, ..., 10^{-1}, 1\}$.
- Since I expect less variation near the optimal dx, evaluate differences of derivatives for adjacent dx values and choose dx corresponding to smallest difference.
- Refine the optimal dx guess by repeating the previous steps above with dx from the interval centered around the best guess $\{dx \cdot 10^-1, ...dx, ...dx \cdot 10\}$. I take the best dx at this point as good enough to proceed.
  - For array inputs of x , the derivative is evaluated at all points of x with all values of dx. Differences between derivatives for adjacent dx values are calculated, then summed along each value of x to get an array of the differences for each dx. The best dx is chosen in the same manner, from the dx corresponding to the minimum difference.

Evaluating the derivative:

- The numerical derivative output is calculated using the central derivative.formula using the chosen best dx at each point in x.

Estimating Error

- Error estimation is calculated according to the formula for the error of the central derivative: $R \approx \frac{f(x)\epsilon}{dx} + \frac{1}{6}f'''(x)dx^2$ where $\epsilon = 10^{-16}$ is the rounding error.
  - The third derivative for the error formula is crudely calculated at each point of the function:
  - For each point in x, I calculate $f'(x \pm 2dx)$ and use these values to get $f''(x + dx) = \frac{f'(x+2dx)-f'(x)}{2dx}$ and $f''(x - dx) = \frac{f'(x)-f'(x-2dx)}{2dx}$. Finally, the value of $f'''(x) = \frac{f''(x+dx)-f''(x-dx)}{2dx}$ is used to evaluate the formula for R.

The code for this question is in the file named "Q2_numerical_differentiator.py". Testing on the function $f(x) = e^x$ results in actual error of order 10^{-11} or lower, and error estimates in the same order of magnitude as the actual error.