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

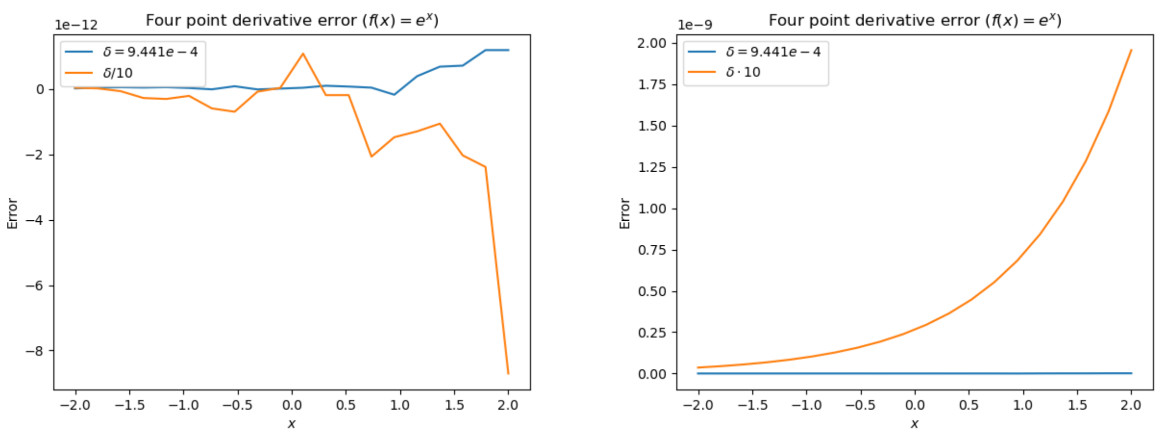
$$\boxed{\delta = \left(\frac{15}{2}\frac{|f(x)| \cdot \epsilon}{f'''''(x)}\right)^{1/5}}.$$

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 $f(x) = e^x$

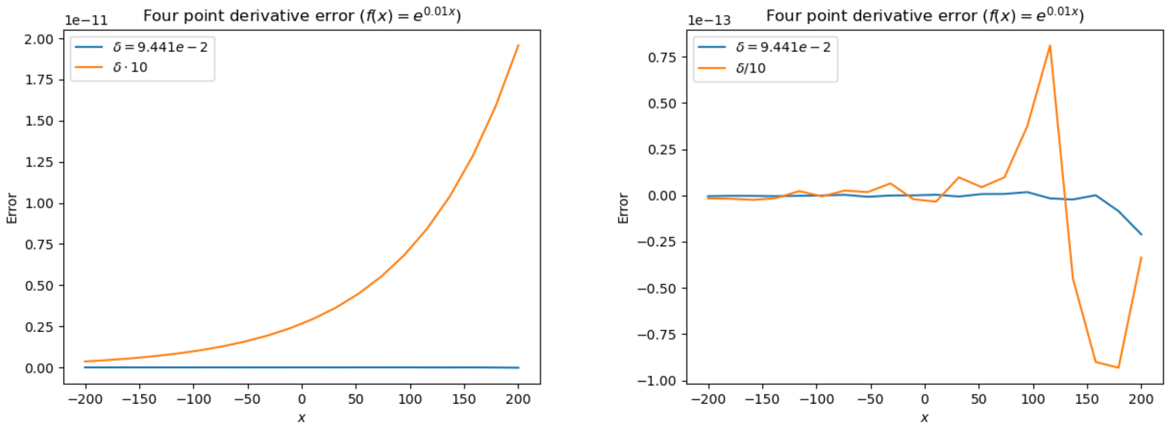


For $f(x) = e^{0.01x}$, the ideal step size should be approximately

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

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 $f(x) = e^{0.01x}$



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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:

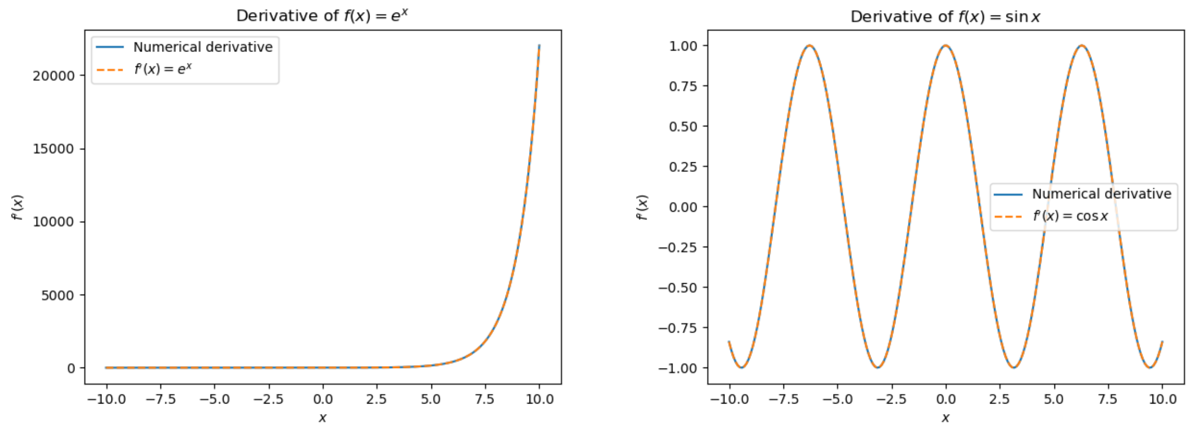
- The numerical derivative output is calculated using the central derivative.formula using the chosen best dx at each point in x.

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. The error estimated by the function is within one order of magnitude to the actual error and generally on the same order of magnitude or even closer. Examples of the function output for e^x and $\sin x$ in Figure 3.

Figure 3: Numerical differentiator sample results



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