PHYS512 A1

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1 Question 1

1.1 Deriving the operator

We can take the derivative of some function $f(x)$ at points $x \pm \delta$ and $x \pm 2\delta$. First dealing with the $x \pm \delta$ points:

$$\hat{f}_1'(x) = \frac{f(x+\delta) - f(x-\delta)}{2\delta} \tag{1}$$

Expanding the right side, we get:

$$\begin{aligned}\hat{f}_1'(x) = \frac{1}{2\delta}\Bigg[&\left(f(x) + \delta f'(x) + \frac{\delta^2}{2!}f''(x) + \frac{\delta^3}{3!}f'''(x) + \frac{\delta^4}{4!}f^{(4)}(x) + \frac{\delta^5}{5!}f^{(5)}(x)\right) \\ &- \left(f(x) - \delta f'(x)\frac{\delta^2}{2!}f''(x) - \frac{\delta^3}{3!}f'''(x) + \frac{\delta^4}{4!}f^{(4)}(x) - \frac{\delta^5}{5!}f^{(5)}(x)\right)\Bigg] + O(\delta^6)\end{aligned} \tag{2}$$

As we can see, several terms cancel and we are left with:

$$\hat{f}_1'(x) = f'(x) + \frac{\delta^2}{3!}f'''(x) + \frac{\delta^4}{5!}f^{(5)}(x) + O(\delta^6) \tag{3}$$

We perform the same computation for the $x \pm 2\delta$ points:

$$\hat{f}_2'(x) = \frac{f(x+2\delta) - f(x-2\delta)}{2(2\delta)} = \frac{f(x+2\delta) - f(x-2\delta)}{4\delta} \tag{4}$$

Expanding the right side and noting that we will have the same terms cancelled as with the $x \pm \delta$ points, we get:

$$\hat{f}_2'(x) = \frac{1}{4\delta}\left[2(2\delta)f'(x) + 2f'''(x)\frac{(2\delta)^3}{3!} + 2\frac{(2\delta)^5}{5!}f^{(5)}(x)\right] + O(\delta^6) \tag{5}$$

We can simplify this to the following:

$$\hat{f}_2'(x) = f'(x) + \frac{2\delta^2}{3}f'''(x) + \frac{2\delta^4}{15}f^{(5)}(x) + O(\delta^6) \tag{6}$$

We can re-arrange the above equation in terms of $f'''(x)$:

$$f'''(x) = \frac{3}{2\delta^2}\left[\hat{f}_2'(x) - f'(x) - \frac{2\delta^4}{15}f^{(5)}(x)\right] + O(\delta^6) \tag{7}$$

We can then substitute (7) into (3) and get:

$$\hat{f}_1'(x) = f'(x) + \frac{\delta^2}{6}\left[\frac{3}{2\delta^2}\left[\hat{f}_2'(x) - f'(x) - \frac{2\delta^4}{15} f^{(5)}(x)\right]\right] + O(\delta^6) \tag{8}$$

Simplifying the resulting expression:

$$\hat{f}_1'(x) = \frac{3}{4} f'(x) - \frac{1}{4}\hat{f}_2'(x) - \frac{\delta^4}{30} f^{(5)}(x) + O(\delta^6) \tag{9}$$

Isolating $f'(x)$ and substituting the definition of a derivative:

$$\begin{aligned} f'(x) &= \frac{4}{3}\hat{f}_1'(x) - \frac{1}{3}\hat{f}_2'(x) - \frac{2\delta^4}{45} f^{(5)}(x) + O(\delta^6) \\ &= \frac{8f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta))}{12\delta} - \frac{2\delta^4}{45} f^{(5)}(x) \\ &\quad + O(\delta^6) \end{aligned} \tag{10}$$

1.2 Deriving the Error

We defined the theoretical error as the difference between the numerical derivative and the analytical derivative.

$$E(x) = \tilde{f}'(x) - f'(x) = \frac{4}{3}\hat{f}_1'(x) - \frac{1}{3}\hat{f}_2'(x) + \phi(\delta^4) - f'(x) \tag{11}$$

We can define the derivative as follows:

$$f'(x) = \lim_{x\to\infty} \frac{f(x+dx) - f(x)}{dx} \tag{12}$$

Taylor expanding the top:

$$f'(x) \approx \frac{[f(x) + f'(x)dx + \frac{f''(x)dx^2}{2}][1 + g_1\epsilon] - f(x)[1 + g_0\epsilon]}{dx} \tag{13}$$

Setting $g = g_1 - g_0$ and collecting like terms:

$$f'(x) \approx \frac{g\epsilon f(x)}{dx} + \frac{f''(x)dx}{2} + \frac{g\epsilon f''(x)dx}{2} + f'(x) \tag{14}$$

We can neglect terms containing ϵdx since they vanish as they are on the order of dx^2:

$$f'(x) \approx \frac{g\epsilon f(x)}{dx} + \frac{f''(x)dx}{2} + f'(x) \tag{15}$$

We can then identify the error as:

$$Err = \frac{g\epsilon f(x)}{dx} + \frac{f''(x)dx}{2} \tag{16}$$

We take the derivative on the other side as well:

$$f'(x) = \lim_{x\to\infty} \frac{f(x) - f(x-dx)}{dx} \tag{17}$$

Performing an expansion:

$$f'(x) \approx \frac{[f(x)[1+g_1\epsilon] - [f(x)+f'(x)dx+\frac{f''(x)dx^2}{2}][1+g_0\epsilon]}{dx} \tag{18}$$

The derivative can be taken on both sides, where

$$\delta_r = \lim_{x\to\infty}\frac{f(x)-f(x-dx)}{dx}, \delta_l = \lim_{x\to\infty}\frac{f(x+dx)-f(x)}{dx} \tag{19}$$

We can get the derivative by averaging these:

$$f'(x) = \frac{\delta_r+\delta_l}{2} = \frac{f(x+dx)-f(x-dx)}{2dx} \tag{20}$$

$$\begin{aligned}\frac{\delta_r+\delta_l}{2} &= \frac{[f(x)+f'(x)dx+\frac{f''(x)dx^2}{2}+\frac{f'''(x)dx^3}{3!}]-[f(x)-f'(x)dx+\frac{f''(x)dx^2}{2}-\frac{f'''(x)dx^3}{3!}]}{2dx}\\ &= \frac{2f'(x)dx+2\frac{f'''(x)dx^3}{3!}}{2dx}\\ &\approx f'(x)+\frac{f'''(x)dx^3}{3!}\end{aligned} \tag{21}$$

Our error then becomes:

$$Err = \frac{g\epsilon f(x)}{dx} + \frac{f'''(x)dx^2}{3!} \tag{22}$$

We differentiate with respect to dx and set to zero:

$$0 = -\frac{g\epsilon f(x)}{dx^2} + \frac{f'''(x)dx}{3} \tag{23}$$

This yields the following expression:

$$dx = \left[\frac{3g\epsilon f(x)}{f'''(x)}\right]^{\frac{1}{3}} \tag{24}$$

If $f \sim f'''$, then $dx \sim \epsilon^{\frac{1}{3}}$. For double precision, we require that $\epsilon \sim 10^{-15}$. In the case of e^x and $e^{0.01x}$, we will plot error as a function of dx with $x = 0$.

2 Question 2

Please refer to the inline comments in the software file.

3 Question 3

The error was approximately calculated by interpolating the derivative of the voltage, taking the derivative of the interpolated voltage, and then finally taking the difference of the two.

4 Question 4

Since the Lorentzian is a rational function, we should theoretically expect a zero error. If we switch from np.linalg.inv to np.linalg.pinv, we get much smaller error. I cannot understand what happened by looking at p and q.

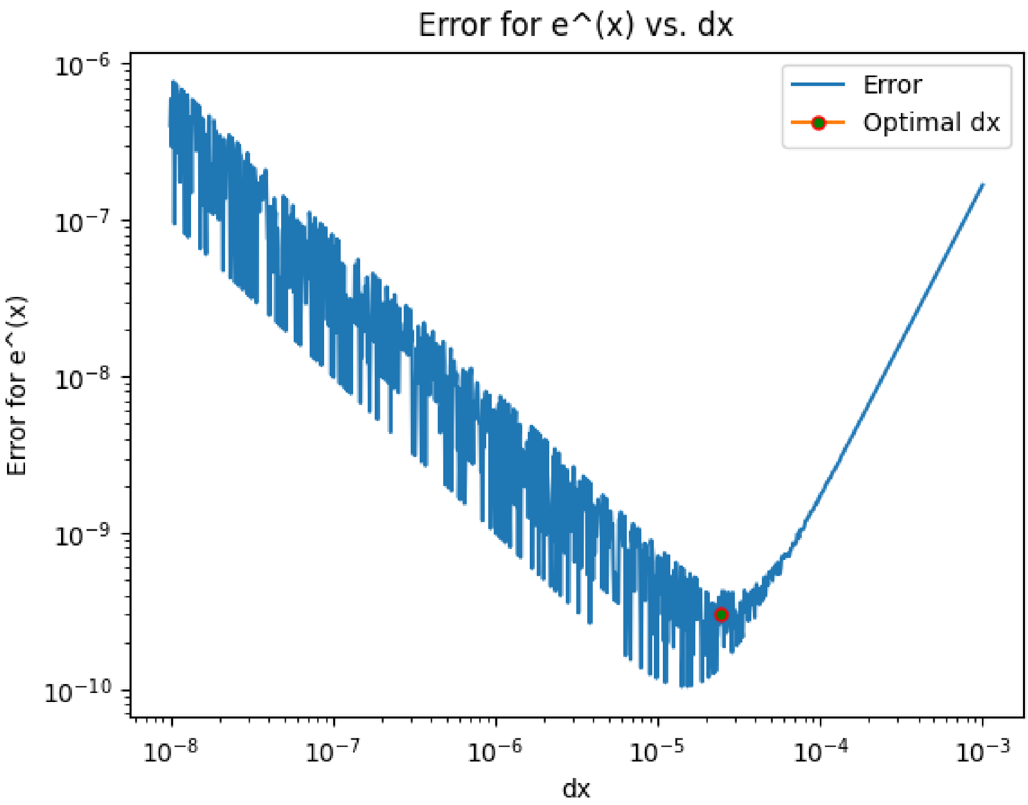

Figure 1: Error for e^x

The x axis is the x value, and the y axis is the error.
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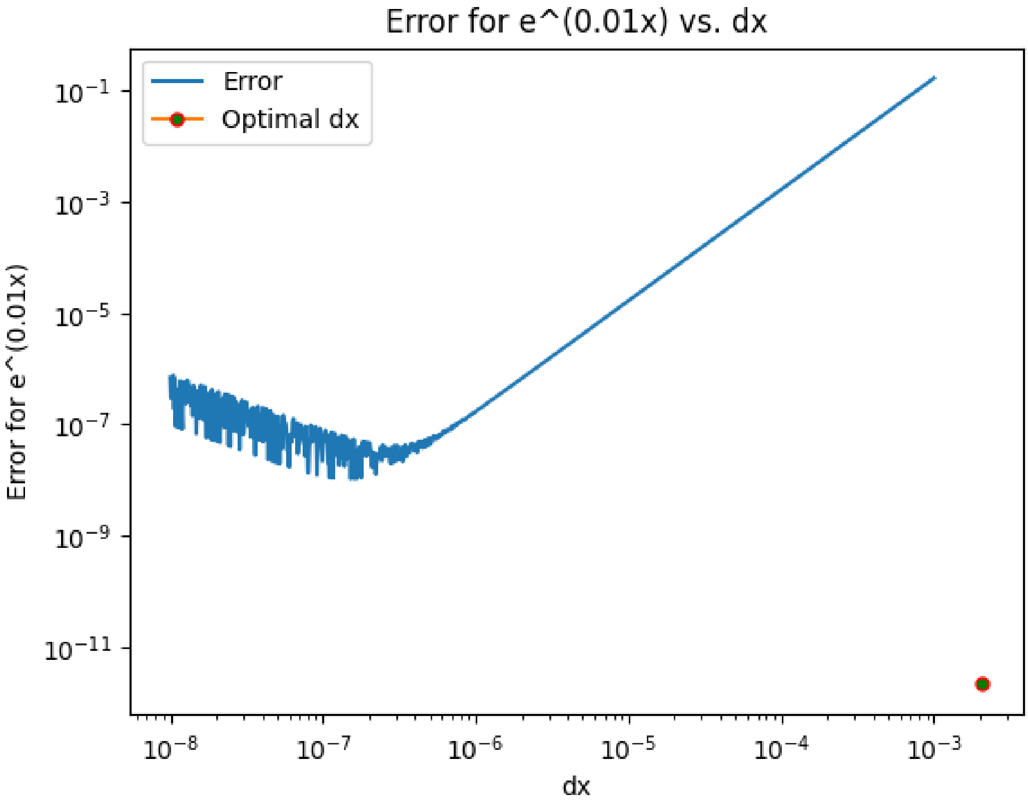

Figure 2: Error for $e^{0.01x}$

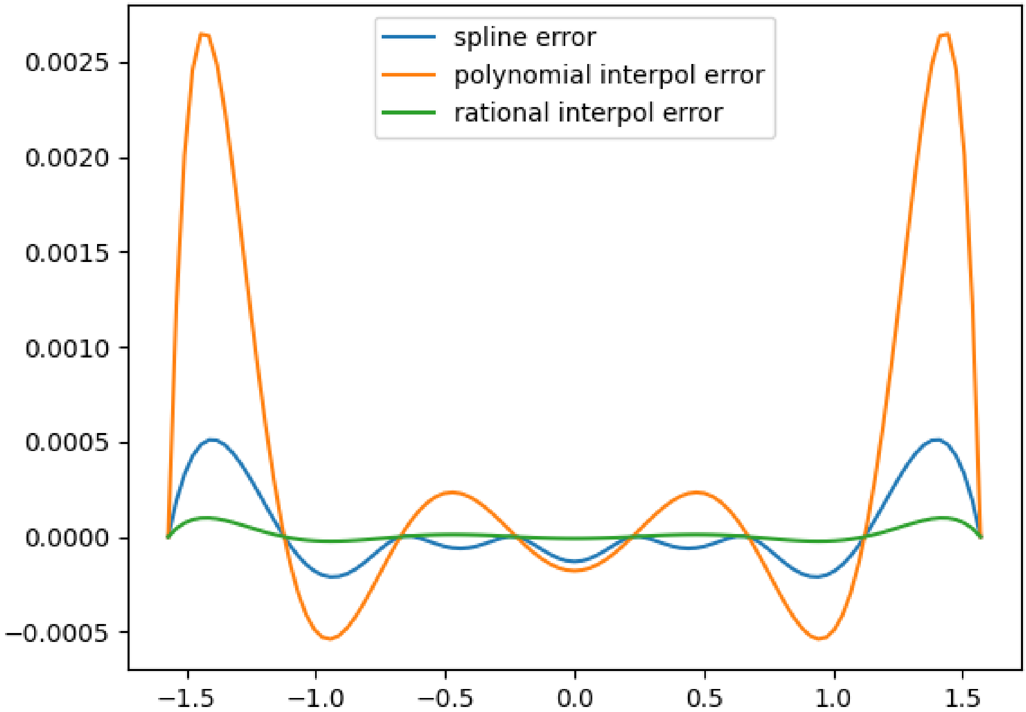

Figure 3: Error for $cos(x)$

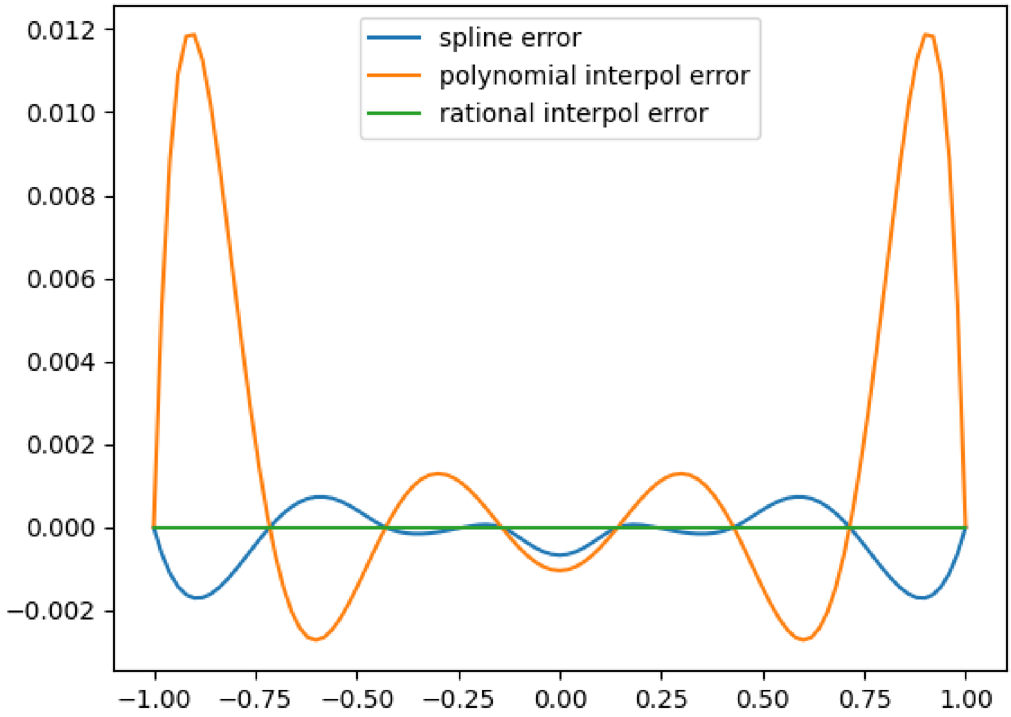

Figure 4: Error for Lorentzian