PHYS338:Computational Physics HW3

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Question 1

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) - \dots$$
(1)

$$f(x-2h) = f(x) - 2hf'(x) + \frac{(2h)^2}{2!}f''(x) - \frac{(2h)^3}{3!}f'''(x) - \dots \quad (2)$$

$$\rightarrow f(x-2h) - 2f(x-h) = -f(x) + h^2 f''(x) - \frac{6h^3}{3!} f'''(x) + \dots \quad (3)$$

$$\to f''(x) = \frac{f(x-2h) - 2f(x-h) + f(x)}{h^2} + hf'''(x) \tag{4}$$

$$\to f''(x) = \frac{f(x-2h) - 2f(x-h) + f(x)}{h^2} \tag{5}$$

Error = h f'''(x) with order 1, that is O(h)

Question 2

I wrote a C code to save all x and y data into 10 text files; 3 methods with 9 texts, each method with 3 different h, and the last text for saving data for the actual derivative function. After saving all data, i used <u>Wolfram Mathematica 12</u> to plot all graphs, and zooming into them until differences between the actual derivative and the numerical derivative functions have been clearly appeared. Now, as we know:

$$\frac{df(x)}{dx} = \frac{d(1 + \tanh x)}{dx} = \operatorname{sech}^2(x) \tag{6}$$

In each of the graphs bellow, there are two curves, one for actual derivative (the blue color curve) and the other for the numerical derivative (the red color curve):

In the first graph -Figure (1)-: Although this is the graph for two points (with h=0.1) that supposed to be the least accurate method, the two curves are much close to each other! So i used Wolfram Mathematica code to zoom in all the remaining graphs with specific scales at the same location. Otherwise, the two curves tend to be the same and the differences cannot be noticed.

In Figure (2), only one curve is noticed, but actually, there is another numerical curve. This is what makes Figure(2) represents all the remaining graphs.

In Figure(4), Figure(5) and Figure(6), all the the graphs have the same zoom scaling at the same location. We can notice that Two points method with h=0.001 is more accurate than Three points with h=0.1!

In the last graph -Figure(11)-, the Five points with h=0.001, does actually represent the exact derivative function as in equation(6), with error \rightarrow zero.



Figure 2: Two points (h=0.01)



Figure 3: Two points Zoom (h=0.1), zooming scale level=0.0195 x center=0.97 , y center=0.425



Figure 4: Two points Zoom (h=0.01), zooming scale level=0.0095 x center=0.97 , y center=0.44



Figure 5: Two points Zoom (h=0.001), zooming scale level=0.0095 x center=0.97 , y center=0.44



Figure 6: Three points Zoom (h=0.1), zooming scale level=0.0095 x center=0.97 , y center=0.44



Figure 7: Three points Zoom (h=0.01), zooming scale level= $5 * 10^{-5}$ x center=0.9696 , y center=0.4397



Figure 8: Three points Zoom (h=0.001), zooming scale level= $5*10^{-7}$ x center=0.9696 , y center=0.439705



Figure 9: Five points Zoom (h=0.1), zooming scale level= $5 * 10^{-4}$ x center=0.9696, y center=0.43995



Figure 10: Five points Zoom (h=0.01), zooming scale level=5 \times 10^{-6} x center=0.9696 , y center=0.439705



Figure 11: Five points Zoom (h=0.001)



Figure 12: The used Wolfram Mathematica Code