PHSX815 HW2 - First Derivative

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The goal here is to study a few different ways to numerically compute the first derivative of a given function and to minimize the error that accompanies the numerical estimation by considering the contributions from the approximations in the expressions for the derivative as well as that due to the machine precision of the system.

Taylor Expansions

The forward and centered difference methods have errors of $\mathcal{O}(h)$ and $\mathcal{O}(h^2)$, respectively, as the centered difference method uses three points as compared to the forward difference method's two. To derive an expression that has an error of $\mathcal{O}(h^4)$, we need to consider five points and compute their Taylor expansions as

$$f(x \pm h) = f(x) \pm f'(x) + \frac{1}{2}f''(x) \pm \frac{1}{6}f'''(x) + \frac{1}{24}f''''(x) + \mathcal{O}(h^5), \tag{1}$$

$$f(x \pm 2h) = f(x) \pm 2f'(x) + 2f''(x) \pm \frac{4}{3}f'''(x) + \frac{2}{3}f''''(x) + \mathcal{O}(h^5). \tag{2}$$

5-point First Derivative

Now, to compute a first derivative with an error of $\mathcal{O}(h^4)$, we can write it as a linear sum of these Taylor expansions as

$$f'(x) = af(x-2h) + bf(x-h) + cf(x) - bf(x+h) - af(x+2h), \tag{3}$$

using symmetry arguments. Here, we need to set the coefficient of $f'(x)$ to be $\frac{1}{h}$ and the rest to be zero. Solving the system of linear equations, we get $a = 1/(12h)$ and $b = -2/(3h)$. This allows us to write the final expression for the five-point first derivative as

$$f'(x) \approx \frac{1}{12h}\left[f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)\right]. \tag{4}$$

Errors

If we compute an additional term (for $f^{(5)}(x)$) in the Taylor expansions for each point and plug that into equation 4, we get

$$f'_{actual}(x) = f'_{numerical}(x) - \frac{1}{30}h^4 f^{(5)}(x) + \mathcal{O}(h^5). \tag{5}$$

Thus, we get the error term to be

$$\epsilon_{truncation} \approx \left(\frac{1}{30}f^{(5)}\right)h^4. \tag{6}$$

This is the error caused due to the approximation of the first derivative and decreases with decreasing step size. However, at a small enough step size, a round-off error kicks in due to the limits of the machine precision of the system ($\approx 2.22 \times 10^{-16}$).

Trial Function

Thus, there exists an optimal step size that reduces the error in the first derivative. To demonstrate this, we look at a trial function

$$f(x) = x^7 \sin x. \tag{7}$$

Empirical Optimal h

We calculate the first derivative of the function given in equation 7 using the five-point approximation 4 and compare it with the analytically calculated first derivative of the function, which is known in this case.

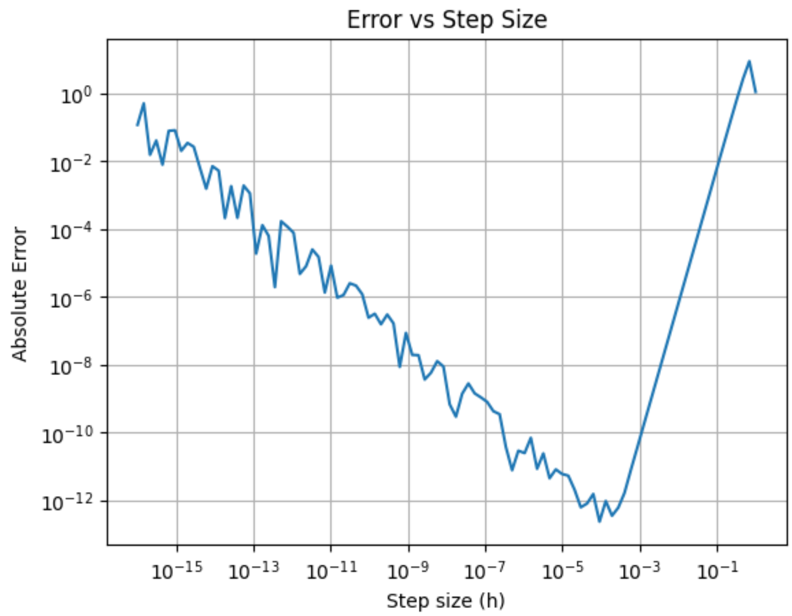

Fig. 1: The error has a minimum at $h \approx 10^{-4}$

We thus get an optimal step size of $h \approx 10^{-4}$.

This can be understood to be arising from the interplay between the magnitudes of the error made by our approximation for the first derivative and that made by the computer due to the limited machine precision.

Round-Off v/s Truncation Errors

We can calculate the total error as the sum of the round-off and truncation errors and compare it with the actual difference between the numerical estimate of the first derivative and the analytically computed first derivative. This gives us a curve that is of the same form as before, but with a near-constant shift, as the exact coefficients of both errors are not taken into consideration.

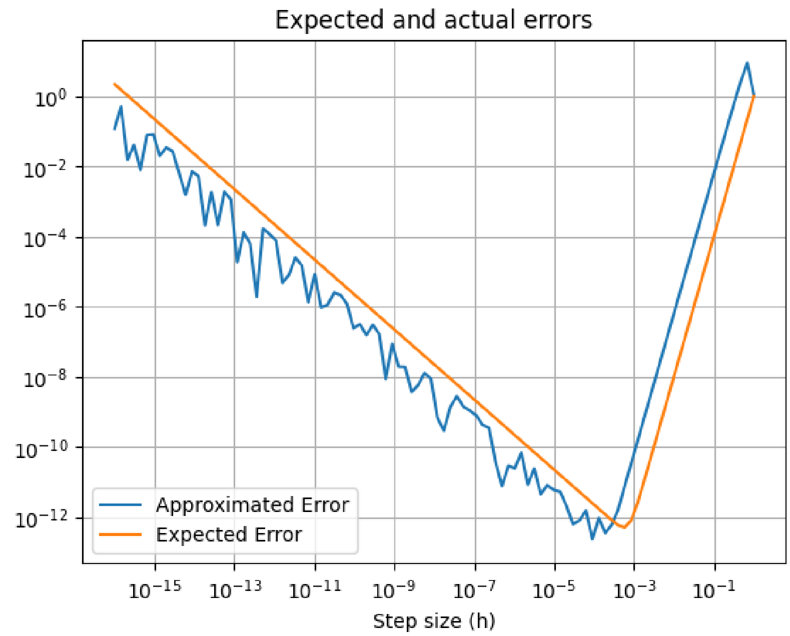

Fig. 2: The optimal step size can be found by equating $\epsilon_{truncation}$ and $\epsilon_{round-off}$, as $h^4 \approx 10^{-16} \Rightarrow h \approx 10^{-4}$

Second Derivative

Using the Taylor expansions in equations 1 and 2, we can similarly calculate approximate expressions for the second derivative as well, with errors of different orders.

Three-Point

Directly adding the two expressions we get from equation 1 allows us to derive a three-point expression for the second derivative with an error of $\mathcal{O}(\langle^{\epsilon})$ as

$$f''(x) \approx \frac{1}{h^2}\left[f(x+h) - 2f(x) + f(x+h)\right]. \tag{8}$$

Five-Point

We can improve this approximation using a five-point expression with an error of $\mathcal{O}(\langle^{\triangle})$, by writing the second derivative as a sum of all four Taylor expanded expressions from equations 1 and 2, setting the coefficient of $f''(x)$ to one and the rest to zero, and solving the system of linear equations thus obtained. This gives us

$$f''(x) \approx \frac{1}{12h^2}\left[-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)\right], \quad (9)$$

which reduces the truncation error made by our numerical approximation.