

7.1: Derivatives

Suppose we have discretized a function of one variable, obtaining a set of $\psi_n \equiv \psi(x_n)$ as described above. For simplicity, we assume that the discretization points are evenly-spaced and arranged in increasing order (this is the simplest and most common discretization scheme). The spacing between points is defined as

$$h \equiv x_{n+1} - x_n. \quad (7.1.1)$$

Let us discuss how the first and higher-order derivatives of $\psi(x)$ can be represented under discretization.

7.1.1 First Derivative

The most straightforward representation of the first derivative is the **forward-difference** formula:

$$\psi'(x_n) \approx \frac{\psi_{n+1} - \psi_n}{h} \quad (7.1.2)$$

This is inspired by the usual definition of the derivative of a function, and approaches the true derivative as $h \rightarrow 0$. However, it is not a very good approximation. To see why, let's analyze the **error** in the formula, which is defined as the absolute value of the difference between the formula and the exact value of the derivative:

$$\mathcal{E} = \left| \psi'(x_n) - \frac{\psi_{n+1} - \psi_n}{h} \right| \quad (7.1.3)$$

We can expand ψ_{n+1} in a Taylor series around x_n :

$$\psi_{n+1} = \psi_n + h \psi'(x_n) + \frac{h^2}{2} \psi''(x_n) + \frac{h^3}{6} \psi'''(x_n) + O(h^4) \quad (7.1.4)$$

Plugging this into the error formula, we find that the error decreases linearly with the spacing:

$$\mathcal{E} = \left| \frac{h}{2} \psi''(x_n) + O(h^2) \right| \sim O(h). \quad (7.1.5)$$

There is a better alternative, called the **mid-point** formula. This approximates the first derivative by sampling the points to the left and right of the desired position:

$$\psi'(x_n) \approx \frac{\psi_{n+1} - \psi_{n-1}}{2h}. \quad (7.1.6)$$

To see why this is better, let us write down the Taylor series for $\psi_{n\pm 1}$:

$$\psi_{n+1} = \psi_n + h \psi'(x_n) + \frac{h^2}{2} \psi''(x_n) + \frac{h^3}{6} \psi'''(x_n) + \frac{h^4}{24} \psi^{(4)}(x_n) + O(h^5) \quad (7.1.7)$$

$$\psi_{n-1} = \psi_n - h \psi'(x_n) + \frac{h^2}{2} \psi''(x_n) - \frac{h^3}{6} \psi'''(x_n) + \frac{h^4}{24} \psi^{(4)}(x_n) + O(h^5) \quad (7.1.8)$$

Note that the two series have the same terms involving even powers of h , whereas the terms involving odd powers of h have opposite signs. Hence, if we subtract the second series from the first, the result is

$$\psi_{n+1} - \psi_{n-1} = 2h \psi'(x_n) + 2 \frac{h^3}{6} \psi'''(x_n) + O(h^5) \quad (7.1.9)$$

Because the $O(h^2)$ terms are equal in the two series, they cancel out under subtraction, and only the $O(h^3)$ and higher terms survive. After re-arranging the above equation, we get

$$\psi'(x_n) = \frac{\psi_{n+1} - \psi_{n-1}}{2h} + O(h^2). \quad (7.1.10)$$

Hence, the error of the mid-point formula scales as $O(h^2)$, which is a good improvement over the $O(h)$ error of the forward-difference formula. What's especially nice is that the mid-point formula requires the same number of arithmetic operations to calculate as the forward-difference formula, so this is a free lunch!

It is possible to come up with better approximation formulas for the first derivative by including terms involving $\psi_{n\pm 2}$ etc., with the goal of canceling the $O(h^3)$ or higher terms in the Taylor series. For most practical purposes, however, the mid-point rule is sufficient.

7.1.2 Second Derivative

The discretization of the second derivative is easy to figure out too. We again write down the Taylor series for $\psi_{n\pm 1}$:

$$\psi_{n+1} = \psi_n + h \psi'(x_n) + \frac{h^2}{2} \psi''(x_n) + \frac{h^3}{6} \psi'''(x_n) + \frac{h^4}{24} \psi''''(x_n) + O(h^5) \quad (7.1.11)$$

$$\psi_{n-1} = \psi_n - h \psi'(x_n) + \frac{h^2}{2} \psi''(x_n) - \frac{h^3}{6} \psi'''(x_n) + \frac{h^4}{24} \psi''''(x_n) + O(h^5) \quad (7.1.12)$$

When we add the two series together, the terms involving odd powers of h cancel, and the result is

$$\psi_{n+1} + \psi_{n-1} = 2\psi_n + h^2 \psi''(x_n) + \frac{h^4}{12} \psi''''(x_n) + O(h^5). \quad (7.1.13)$$

A minor rearrangement of the equation then gives

$$\psi''(x_n) \approx \frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{h^2} + O(h^2). \quad (7.1.14)$$

This is called the **three-point rule** for the second derivative, because it involves the value of the function at the three points x_{n+1} , x_n , and x_{n-1} .

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