

Lecture 8 – Numerical Analysis 2

High-Order Numerical Derivation:

In this section, we will discuss how to estimate the second-order derivative numerically. Let's assume that a function $f(x)$ is continuous and continuously differentiable on an interval $[x - \Delta x, x + \Delta x]$. In this case, we can use what's called the **Taylor Expansion** to derive an estimated formula for the second derivative of the function $f(x)$. The Taylor series expansion is given as:

$$f(x + \Delta x) = f(x) + \Delta x f'(x) + \frac{(\Delta x)^2}{2!} f''(x) + \frac{(\Delta x)^3}{3!} f'''(x) + \frac{(\Delta x)^4}{4!} f''''(x) + \dots$$

$$f(x - \Delta x) = f(x) + (-\Delta x) f'(x) + \frac{(-\Delta x)^2}{2!} f''(x) + \frac{(-\Delta x)^3}{3!} f'''(x) + \frac{(-\Delta x)^4}{4!} f''''(x) + \dots$$

$$\Rightarrow f(x - \Delta x) = f(x) - \Delta x f'(x) + \frac{(\Delta x)^2}{2!} f''(x) - \frac{(\Delta x)^3}{3!} f'''(x) + \frac{(\Delta x)^4}{4!} f''''(x) + \dots$$

Now, by adding the two equations above $f(x + \Delta x) + f(x - \Delta x)$, we obtain:

$$f(x + \Delta x) + f(x - \Delta x) = 2f(x) + 2 \frac{(\Delta x)^2}{2!} f''(x) + 2 \frac{(\Delta x)^4}{4!} f''''(x) + \dots$$

$$\Rightarrow f(x + \Delta x) + f(x - \Delta x) = 2f(x) + (\Delta x)^2 f''(x) + O((\Delta x)^4)$$

$$\Rightarrow f''(x) = \frac{f(x + \Delta x) + f(x - \Delta x) - 2f(x)}{(\Delta x)^2} - \frac{O((\Delta x)^4)}{(\Delta x)^2}$$

$$\Rightarrow f''(x) = \frac{f(x + \Delta x) + f(x - \Delta x) - 2f(x)}{(\Delta x)^2} - O((\Delta x)^2)$$

$$\Rightarrow f''(x) = \frac{f(x + \Delta x) + f(x - \Delta x) - 2f(x)}{(\Delta x)^2} \dots (4)$$

The last formula (Equation 4) is the one we will use to estimate the second derivative of the function $f(x)$. The error that we will

encounter when estimating the second derivative is equal to $O((\Delta x)^2)$.

Example:

Estimate the value of the second derivative of the function

$f(x) = 2e^{1.5x}$, and then calculate the absolute and relative error of the estimate.

Solution: Applying Equation 4 above with $\Delta x = 0.1$ and $x=3$:

$$\begin{aligned}
f'(x=3) &\approx \frac{f(x+\Delta x) + f(x-\Delta x) - 2f(x)}{(\Delta x)^2} \\
&= \frac{f(3+0.1) + f(3-0.1) - 2f(3)}{(0.1)^2} \\
&= \frac{f(3.1) + f(2.9) - 2f(3)}{0.01} \\
&= \frac{2e^{1.5(3.1)} + 2e^{1.5(2.9)} - 2(2e^{1.5(3)})}{0.01} = 405.8373
\end{aligned}$$

The estimated value of the second derivative is (405.8372). when $\Delta x = 0.1$ and $x=3$

The true value of the second derivative is:

$$\begin{aligned}
f'(x) &= 2 \frac{d}{dx} e^{1.5x} \\
&= 2(1.5e^{1.5x}) = 3e^{1.5x}
\end{aligned}$$

$$f'(x=3) = 4.5e^{1.5 \times 3} = 405.0771$$

As can be observed, the estimated value is very close to the true value of the second derivative.

In this case, the absolute error is calculated as follows:

$$\text{AbsoluteError} = |405.0771 - 405.8372| = 0.7601$$

Homework:

Estimate the value of the second derivative of the following function when $x=2, \Delta x = 0.1$:

$$f(x) = \ln(2x - 1)$$

Then, find the absolute error of the estimated solution compared to the real solution, noting that the second real derivative is:

$$f''(x) = \frac{-4}{(2x - 1)^2}$$