

Central Divided Difference Approximation of First Derivative of a Function An Example to Answer The Big Oh Mystery

Many students are challenged to understand the nature of Big Oh in relating it to the order of accuracy of numerical methods. In this exercise, we are using the central divided difference approximation of the first derivative of the function to ease some of the mystery surrounding the Big Oh.

Using

$$x_{i-1} = x_i - \Delta x,$$

$$x_{i+1} = x_i + \Delta x,$$

from the Taylor series

$$\begin{aligned} f(x_{i+1}) &= f(x_i) + f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 \\ &\quad + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \frac{f''''(x_i)}{4!}(\Delta x)^4 \\ &\quad + \frac{f'''''(x_i)}{5!}(\Delta x)^5 + \dots \end{aligned} \quad (1)$$

and

$$\begin{aligned} f(x_{i-1}) &= f(x_i) - f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 \\ &\quad - \frac{f'''(x_i)}{3!}(\Delta x)^3 + \frac{f''''(x_i)}{4!}(\Delta x)^4 \\ &\quad - \frac{f'''''(x_i)}{5!}(\Delta x)^5 + \dots \end{aligned} \quad (2)$$

Subtracting Equation (2) from Equation (1)

$$\begin{aligned} f(x_{i+1}) - f(x_{i-1}) &= f'(x_i)(2\Delta x) + \frac{2f'''(x_i)}{3!}(\Delta x)^3 \\ &\quad + \frac{2f'''''(x_i)}{5!}(\Delta x)^5 + \dots \\ f(x_{i+1}) - f(x_{i-1}) - \frac{2f'''(x_i)}{3!}(\Delta x)^3 & \\ - \frac{2f'''''(x_i)}{5!}(\Delta x)^5 - \dots &= f'(x_i)(2\Delta x) \end{aligned}$$

$$\begin{aligned} f'(x_i)(2\Delta x) &= f(x_{i+1}) - f(x_{i-1}) \\ &\quad - \frac{2f'''(x_i)}{3!}(\Delta x)^3 - \frac{2f'''''(x_i)}{5!}(\Delta x)^5 - \dots \end{aligned}$$

$$\begin{aligned} f'(x_i) &= \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} \\ &\quad - \frac{f'''(x_i)}{3!}(\Delta x)^2 - \frac{f'''''(x_i)}{5!}(\Delta x)^4 - \dots \end{aligned}$$

$$= \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + O(\Delta x)^2$$

hence showing that the true error is of the order of $O(\Delta x)^2$ as the true error is given by

$$E_t = -\frac{f'''(x_i)}{3!}(\Delta x)^2 - \frac{f''''(x_i)}{5!}(\Delta x)^4 - \dots$$

Take the example of being asked to find the approximate value of the first derivative of $2e^{1.5x}$ at $x=3$ using central divided difference scheme. The exact value (up to 5 significant digits) using differential calculus is found to be =270.05. Let us find the central divided difference approximation of the first derivative with $\Delta x = 0.1$ and then continue halving the step size.

Δx	Central Divided Difference Approximation $\frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x}$	True Error= Exact Value – Approximate Value
0.1	271.07	-1.0138
0.05	270.30	-0.25324
0.025	270.11	-0.06330
0.0125	270.06	-0.015824
0.00625	270.05	-0.0039558

Δx	First Term of Error $-\frac{f'''(x_i)}{3!}(\Delta x)^2$	Rest of the True Error $-\frac{f''''(x_i)}{5!}(\Delta x)^4 - \frac{f''''''(x_i)}{7!}(\Delta x)^6 - \dots$	True Error divided by $(\Delta x)^2$
0.1	-1.0127	-1.1399×10^{-3}	-101.38
0.05	-0.25317	-7.1216×10^{-5}	-101.30
0.025	-0.063293	-4.4520×10^{-6}	-101.27
0.0125	-0.015823	-2.7970×10^{-7}	-101.27
0.00625	-0.0039556	-1.8955×10^{-8}	-101.27

As you are able to see that the magnitude of the first term of the true error is much bigger than the magnitude of the rest of the true error terms and hence dominates the magnitude of the true error. Note that the value of the true error divided by $(\Delta x)^2$ also gets close to being a constant as Δx

becomes smaller. In fact, the value would converge to the coefficient term of $(\Delta x)^2$ in the true error term,

$$-\frac{f'''(3)}{3!} = -101.27$$

(for $f(x) = 2e^{1.5x}$, $f'''(x) = 6.750e^{1.5x}$).