Numerical Differentiation

Numerical Differentiation is a method used to approximate the value of a derivative over a continuous region [a,b].

Let f(x) is a continuous function with step size h. There are forward, backward and centered difference methods to approximate the derivatives of f(x) at a point x_i.

5.1 Forward Difference Approximation of the First Derivative

We know

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

For a finite $'\Delta x'$.

$$f'(x) \cong \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

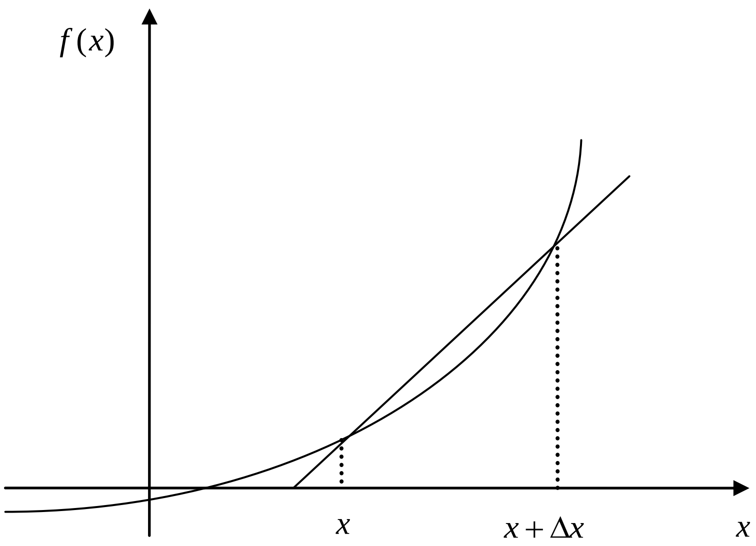

Figure 5.1: Graphical representation of forward difference approximation of first derivative

So if you want to find the value of $f'(x)$ at $x = x_i$, we may choose another point $'\Delta x'$ ahead as $x = x_{i+1}$. This gives

$$\boxed{f'(x_i) \cong \frac{f(x_{i+1}) - f(x_i)}{\Delta x}}$$

$$= \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \qquad \text{Where } \Delta x = x_{i+1} - x_i$$

Example 5.1

The velocity of a rocket is given by $v(t)=2000\ln\left[\frac{14\times10^4}{14\times10^4-2100t}\right]-9.8t \quad , \quad 0\le t\le 30$

Where $'v'$ is given in m/s and $'t'$ is given in seconds.

Use forward difference approximation of the first derivative of $v(t)$ to calculate the acceleration at $t=16s$. Use a step size of $\Delta t=2s$.

Solution

$$a(t_i)\cong\frac{v(t_{i+1})-v(t_i)}{\Delta t}$$

$t_i=16$

$\Delta t=2$

$t_{i+1}=t_i+\Delta t=16+2=18$

$$a(16)=\frac{v(18)-v(16)}{2}$$

$$v(18)=2000\ln\left[\frac{14\times10^4}{14\times10^4-2100(18)}\right]-9.8(18)=453.02m/s$$

$$v(16)=2000\ln\left[\frac{14\times10^4}{14\times10^4-2100(16)}\right]-9.8(16)=392.07m/s$$

Hence

$$a(16)=\frac{v(18)-v(16)}{2}=\frac{453.02-392.07}{2}=30.475m/s^2$$

The exact value of $a(16)$ can be calculated by differentiating

$$a(t)=\frac{d}{dt}\left[2000\ln\left[\frac{14\times10^4}{14\times10^4-2100\,t}\right]-9.8t\right] \quad =2000\left(\frac{14\times10^4-2100\,t}{14\times10^4}\right)\frac{d}{dt}\left(\frac{14\times10^4}{14\times10^4-2100\,t}\right)-9.8$$

$$=2000\left(\frac{14\times10^4-2100\,t}{14\times10^4}\right)(-1)\left(\frac{14\times10^4}{(14\times10^4-2100\,t)^2}\right)(-2100)-9.8 \quad =29.674m/s^2$$

The absolute relative true error is

$$|\in_t|=\left|\frac{\text{True Value - Approximate Value}}{\text{True Value}}\right|\times100=\left|\frac{29.674-30.475}{29.674}\right|\times100=2.6993\%$$

5.2 Backward Difference Approximation of the First Derivative

We know

$$f'(x) = \lim_{\Delta x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

For a finite $'\Delta x'$,

$$f'(x) \cong \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

If $'\Delta x'$ is chosen as a negative number,

$$f'(x) \cong \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

$$f'(x) = \frac{f(x) - f(x-\Delta x)}{\Delta x}$$

This is a backward difference approximation as you are taking a point backward from x. To find the value of $f'(x)$ at $x = x_i$, we may choose another point $'\Delta x'$ behind as $x = x_{i-1}$. This gives

$$\boxed{f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{\Delta x}}$$

$$= \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \quad \text{where} \quad \Delta x = x_i - x_{i-1}$$

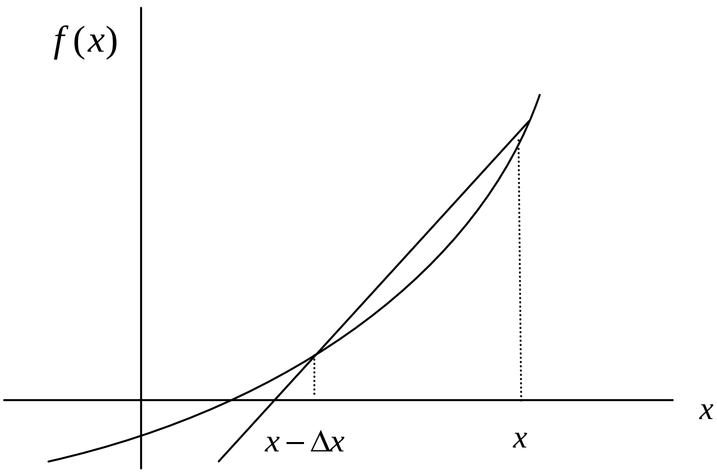

Figure 5.2 Graphical representation of backward difference approximation of first derivative

Example 5.2

The velocity of a rocket is given by

$$\nu(t) = 2000 \ln\left[\frac{14\times10^4}{14\times10^4 - 2100\,t}\right] - 9.8t \ ,\ 0 \le t \le 30$$

Use backward difference approximation of the first derivative of $\nu(t)$ to calculate the acceleration at $t = 16s$. Use a step size of $\Delta t = 2s$.

Solution

$$a(t) \cong \frac{\nu(t_i) - \nu(t_{i-1})}{\Delta t}$$

$$t_i = 16$$

$$\Delta t = 2$$

$$t_{i-1} = t_i - \Delta t = 16 - 2 = 14$$

$$a(16) = \frac{\nu(16) - \nu(14)}{2}$$

$$\nu(16) = 2000 \ln\left[\frac{14\times10^4}{14\times10^4 - 2100(16)}\right] - 9.8(16) = 392.07 m/s$$

$$\nu(14) = 2000 \ln\left[\frac{14\times10^4}{14\times10^4 - 2100(14)}\right] - 9.8(14) = 334.24 m/s$$

$$a(16) = \frac{\nu(16) - \nu(14)}{2} = \frac{392.07 - 334.24}{2} = 28.915 m/s^2$$

The absolute relative true error is

$$|\epsilon_t| = \left|\frac{29.674 - 28.915}{29.674}\right| \times 100 \quad = 2.557\%$$

5.3 Central Difference Approximation of the First Derivative

As shown above, both forward and backward divided difference approximation of the first derivative are accurate on the order of $0(\Delta x)$. Can we get better approximations?

Yes, another method to approximate the first derivative is called the **Central difference approximation of the first derivative.**

From Taylor series

$$f(x_{i+1}) = f(x_i) + f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \text{K} \qquad (1)$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 - \frac{f'''(x_i)}{3!}(\Delta x)^3 + \text{K} \qquad (2)$$

Subtracting equation (2) from equation (1)

$$f(x_{i+1}) - f(x_{i-1}) = f'(x_i)(2\Delta x) + \frac{2f'''(x_i)}{3!}(\Delta x)^3 + \text{K}$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} - \frac{f'''(x_i)}{3!}(\Delta x)^2 + \text{K}$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + 0(\Delta x)^2$$

$$\boxed{f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x}}$$

Hence showing that we have obtained a more accurate formula as the error is of the order of $0(\Delta x)^2$.

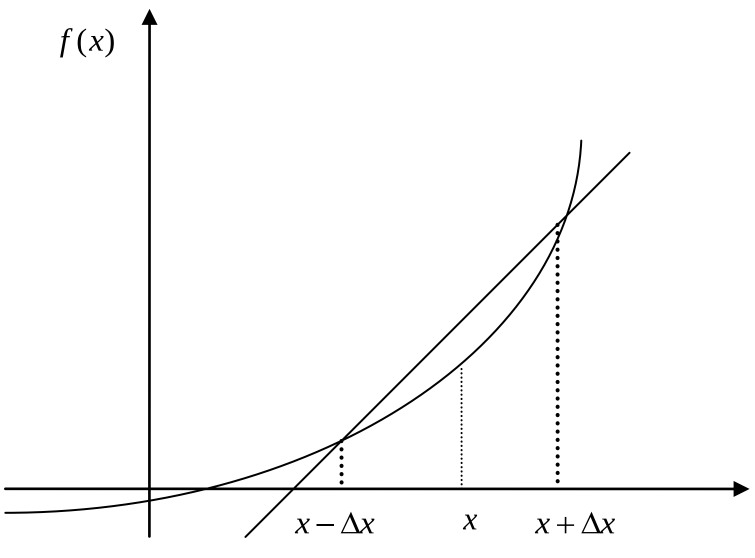

Figure 5.3 Graphical Representation of central difference approximation of first derivative.

Example 5.3

The velocity of a rocket is given by

$$v(t) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t, 0 \le t \le 30.$$

Use central divided difference approximation of the first derivative of $v(t)$ to calculate the acceleration at $t = 16s$. Use a step size of $\Delta t = 2s$.

Solution

$$a(t_i) \cong \frac{v(t_{i+1}) - v(t_{i-1})}{2\Delta t}$$

$$t_i = 16$$

$$t_{i+1} = t_i + \Delta t = 16 + 2 = 18$$

$$t_{i-1} = t_i - \Delta t = 16 - 2 = 14$$

$$a(16) = \frac{v(18) - v(14)}{2(2)} = \frac{v(18) - v(14)}{4}$$

$$v(18) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(18)}\right] - 9.8(18) = 453.02 m/s$$

$$v(14) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(14)}\right] - 9.8(14) = 334.24 m/s$$

$$a(16) = \frac{v(18) - v(14)}{4} = \frac{453.02 - 334.24}{4} = 29.695 m/s^2$$

The absolute relative true error is

$$|\in_t| = \left|\frac{29.674 - 29.695}{29.674}\right| \times 100 = 0.070769\%$$

The results from the three difference approximations are given in Table 1.

Table 1 Summary of $a(16)$ using different divided difference approximations.

Type of Difference Approximation	$a(16)$ (m/s^2)	$\|\in_t\|\%$
Forward	30.475	2.6993
Backward	28.915	2.557
Central	29.695	0.070769

Clearly, the central difference scheme is giving more accurate results because the order of accuracy is proportional to the square of the step size.

5.4 Higher Order Derivatives

Example: Second order derivative:

Note that for the centered formulation, it is a derivation of a derivative:

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

Forward $\quad f''(x) \cong \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2}$

Backward $\quad f''(x) \cong \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{(\Delta x)^2}$

Centered $\quad f''(x) \cong \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(\Delta x)^2}$

I) Forward Difference Methods

First Derivative

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x}$$

Second Derivative

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

Third Derivative

$$f^{(3)}(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{(\Delta x)^3}$$

Fourth Derivative

$$f^{(4)}(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{(\Delta x)^4}$$

II) Backward Difference Methods

First Derivative

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{\Delta x}$$

Second Derivative

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

Third Derivative

$$f^{(3)}(x_i) = \frac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{(\Delta x)^3}$$

Fourth Derivative

$$f^{(4)}(x_i) = \frac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{(\Delta x)^4}$$

III) Central Difference Methods

First Derivative

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

Second Derivative

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

Third Derivative

$$f^{(3)}(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2(\Delta x)^3}$$

Fourth Derivative

$$f^{(4)}(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{(\Delta x)^4}$$