# Numerical Differentiation

## 1. Differentiation of Continuous Functions

The derivative of a function at $x$ is defined as

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

To be able to find a derivative numerically, one could make $\Delta x$ finite to give,

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

Knowing the value of $x$ at which you want to find the derivative of $f(x)$, we choose a value of $\Delta x$ to find the value of $f'(x)$. To estimate the value of $f'(x)$, three such approximations are suggested as follows.

## 2.1 Forward Difference Approximation of the First Derivative

From differential calculus, we know

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

For a finite $\Delta x$,

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

The above is the forward divided difference approximation of the first derivative. It is called forward because you are taking a point ahead of $x$. 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

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

where $\Delta x = x_{i+1} - x_i$.

**Example 7.1:** The velocity of a rocket is given by

$$v(t) = 2000 \ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100t}\right] - 9.8t,\ 0 \le t \le 30,$$

where $v$ is given in m/s and $t$ is given in seconds. At $t = 16$ s,

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

b) find the exact value of the acceleration of the rocket.

c) calculate the absolute relative true error for part (b).

**Solution:**

(a) $a(t_i) \approx \frac{v(t_{i+1}) - v(t_i)}{\Delta t}$ , $t_i = 16$ , $\Delta t = 2$ , $t_{i+1} = t_i + \Delta t$ =16+2=18.

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

$$v(18) = 2000 \ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100(18)}\right] - 9.8(18) = 453.02 \text{ m/s} ,$$

$$v(16) = 2000 \ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100(16)}\right] - 9.8(16) = 392.07 \text{ m/s} .$$

Hence

$$a(16) \approx \frac{v(18) - v(16)}{2} = \frac{453.02 - 392.07}{2} = 30.474 \text{ m/s}^2 .$$

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

$$v(t) = 2000 \ln\left[\frac{14\times 10^4}{14\times 10^4 - 2100t}\right] - 9.8t \quad \text{as} \quad a(t) = \frac{d}{dt}[v(t)] .$$

Knowing that

$$\frac{d}{dt}[\ln(t)] = \frac{1}{t} \text{ and } \frac{d}{dt}\left[\frac{1}{t}\right] = -\frac{1}{t^2} .$$

$$a(t) = 2000\left(\frac{14\times 10^4 - 2100t}{14\times 10^4}\right)\frac{d}{dt}\left(\frac{14\times 10^4}{14\times 10^4 - 2100t}\right) - 9.8$$

$$= 2000\left(\frac{14\times 10^4 - 2100t}{14\times 10^4}\right)(-1)\left(\frac{14\times 10^4}{(14\times 10^4 - 2100t)^2}\right)(-2100) - 9.8$$

$$= \frac{-4040 - 29.4t}{-200 + 3t} .$$

$$a(16) = \frac{-4040 - 29.4(16)}{-200 + 3(16)} = 29.674 \text{ m/s}^2 .$$

(c) The absolute relative true error is

$$|\in_t| = \left|\frac{\text{True Value} - \text{Approximate Value}}{\text{True Value}}\right| \times 100 = \left|\frac{29.674 - 30.474}{29.674}\right| \times 100 = 2.6967 \% .$$

## 2.2 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 $\Delta x$ ,

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

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

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

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

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

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

**2.3 Forward Difference Approximation from Taylor Series**

Taylor's theorem says that if you know the value of a function $f(x)$ at a point $x_i$ and all its derivatives at that point, provided the derivatives are continuous between $x_i$ and $x_{i+1}$, then

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

Substituting for convenience $\Delta x = x_{i+1} - x_i$

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

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

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

The $O(\Delta x)$ term shows that the error in the approximation is of the order of $\Delta x$.

Can you now derive from the Taylor series the formula for the backward divided difference approximation of the first derivative?

As you can see, both forward and backward divided difference approximations of the first derivative are accurate on the order of $O(\Delta x)$. Can we get better approximations? Yes, another method to approximate the first derivative is called the **central difference approximation of the first derivative.**

From the Taylor series

$$f(x_{i+1}) = f(x_i) + f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \ldots \qquad (7.1)$$

and

$$f(x_{i-1}) = f(x_i) - f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 - \frac{f'''(x_i)}{3!}(\Delta x)^3 + \ldots \qquad (7.2)$$

Subtracting Equation (7.2) from Equation (7.1)

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

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

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

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

**Example 7.3:** The velocity of a rocket is given by

$$v(t) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t}\right] - 9.8t, 0 \le t \le 30.$$

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

(b) Find the absolute relative true error for part (a).

**Solution:** $a(t_i) \approx \frac{v(t_{i+1}) - v(t_{i-1})}{2\Delta t}$, $t_i = 16$, $\Delta t = 2$, $t_{i+1} = t_i + \Delta t = 16 + 2 = 18$,

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

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

$$v(18) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)}\right] - 9.8(18) = 453.02 \text{ m/s},$$

$$v(14) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(14)}\right] - 9.8(14) = 334.24 \text{ m/s}.$$

Hence

$$a(16) \approx \frac{v(18) - v(14)}{4} = \frac{453.02 - 334.24}{4} = 29.694 \text{ m/s}^2.$$

(b) The exact value of the acceleration at $t = 16$ s from Example 7.1 is

$$a(16) = 29.674 \text{ m/s}^2.$$

The absolute relative true error for the answer in part (a) is

$$|\in_t| = \left|\frac{29.674 - 29.694}{29.674}\right| \times 100 = 0.069157 \ \% .$$

The results from the three difference approximations are given in Table 7.1.

**Table 7.1** Summary of $a(16)$ using different difference approximations.

| Type of difference approximation | $a(16)$ $(\mathrm{m/s}^2)$ | $\|\in_t\|\%$ |
|---|---|---|
| Forward | 30.475 | 2.6967 |
| Backward | 28.915 | 2.5584 |
| Central | 29.695 | 0.069157 |

Clearly, the central difference scheme is giving more accurate results because the order of accuracy is proportional to the square of the step size. In real life, one would not know the exact value of the derivative – so how would one know how accurately they have found the value of the derivative? A simple way would be to start with a step size and keep on halving the step size until the absolute relative approximate error is within a pre-specified tolerance.

Take the example of finding $v'(t)$ for

$$v(t) = 2000 \ln\left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t}\right] - 9.8t ,$$

at $t = 16$ using the backward difference scheme. Given in Table 7.2 are the values obtained using the backward difference approximation method and the corresponding absolute relative approximate errors.

**Table 7.2** First derivative approximations and relative errors for different $\Delta t$ values of backward difference scheme.

| $\Delta t$ | $v'(t)$ | $\|\in_a\|\%$ |
|---|---|---|
| 2 | 28.915 | |
| 1 | 29.289 | 1.2792 |
| 0.5 | 29.480 | 0.64787 |
| 0.25 | 29.577 | 0.32604 |
| 0.125 | 29.625 | 0.16355 |

From the above table, one can see that the absolute relative approximate error decreases as the step size is reduced. At $\Delta t = 0.125$ , the absolute relative approximate error is 0.16355%, meaning that at least 2 significant digits are correct in the answer.

**3 Differentiation of Discrete Functions**

If we are given the set of distinct points $(x_i, y_i)$, $i = 0, 1, 2, ..., n$, determine the interpolation polynomial passing through these points. We then differentiate this polynomial to obtain $p^{(j)}(x)$ , *j*=1, 2, … whose values for any given x taken as an approximation to $f^{(j)}(x)$ . Construct a polynomial $p_n(x)$ which is best approximate polynomial to *f*(*x*) by any methods given in interpolation.

**Note** 7.1**:**

1) For unequally space points we must use Lagrange interpolation polynomial, divided difference interpolation formula.
2) For equally space points, we able to use all available methods in interpolation.
3) If we find $p_n(x)$ by Lagrange interpolation polynomial, divided difference interpolation formula or spline function, differentiate $p_n(x)$ with respect to *x* directly.
4) If we find $p_n(x)$ by NFDIF, NBDIF, we differentiate $p_n(x)$ with respect to *x* as follows.

$$\frac{df(x)}{dx} \cong \frac{dp_n(x)}{dx} = \frac{dp_n(x)}{ds}\frac{ds}{dx} = \frac{1}{h}\frac{dp_n(x)}{ds}$$

$$= \frac{1}{h}\frac{d}{ds}\left\{ y_0 + s\Delta y_0 + \frac{s(s-1)}{2!}\Delta^2 y_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 y_0 + \cdots \right\}$$

$$= \frac{1}{h}\left\{ \Delta y_0 + (s - \frac{1}{2})\Delta^2 y_0 + (\frac{s^2}{2} - s + \frac{1}{3})\Delta^3 y_0 + \cdots \right\}.$$

$$\frac{d^2 f(x)}{dx^2} \cong \frac{d^2 p_n(x)}{dx^2} = \frac{d}{dx}\left[ \frac{1}{h}\left\{ \Delta y_0 + (s - \frac{1}{2})\Delta^2 y_0 + (\frac{s^2}{2} - s + \frac{1}{3})\Delta^3 y_0 + \cdots \right\} \right]$$

$$= \frac{d}{ds}\left[ \frac{1}{h}\left\{ \Delta y_0 + (s - \frac{1}{2})\Delta^2 y_0 + (\frac{s^2}{2} - s + \frac{1}{3})\Delta^3 y_0 + \cdots \right\} \right]\frac{ds}{dx}$$

$$= \frac{1}{h^2}\left\{ \Delta^2 y_0 + (s-1)\Delta^3 y_0 + \cdots \right\}.$$

In general

$$\frac{d^j f(x)}{dx^j} \cong \frac{d^j p_n(x)}{dx^j} = \frac{1}{h^j}\frac{d^j p_n(x)}{ds^j},\ j=1, 2, \dots .$$

Similarly, we obtain $\frac{d^j f(x)}{dx^j} \cong \frac{d^j p_n(x)}{dx^j}$ for Newton backward difference interpolation and Bessel's interpolation formula.

**Note** 7.2**:** If $x=x_i$ (interpolation point)$\Rightarrow s=0$.

**Example** 7.**6:** Find an approximate value to $f'(0.7)$ where $f(x)=\sin(x)$ and $x_0=0.4$, $x_1=0.6$, $x_2=0.8$, $x_3=1$.

**Solution:**

| $x$ | 0.4 | 0.6 | 0.8 | 1 |
|---|---|---|---|---|
| $f(x)$ | 0.389418 | 0.564642 | 0.717356 | 0.841471 |

By using LIP,

$x_0=0.4$, $x_1=0.6$, $x_2=0.8$, $x_3=1$, $y_0=0.389418$, $y_1=0.564642$,

$y_2=0.717356$, $y_3=0.841471$.

$$p_3(x)=\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}y_0+\frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}y_1+$$

$$\frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_1-x_3)}y_2+\frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}y_3$$

$$=-0.12683772\,x^3-0.05307353\,x^2+1.02559085\,x-0.00420862\,.$$

Hence

$$\Rightarrow\ p_3'(x)=-0.38051316\,x^2-0.10614706\,x+1.02559085$$

$$\Rightarrow\ f'(0.7)\cong p_3'(0.7)=0.7648346\,.$$

Exact value=cos(0.7)=0.76484219$\Rightarrow$ error=0.00000573.

**Example** 7.**7:** Find an approximate value to $f'(2.31)$ and $f'(1)$ by using Newton forward difference interpolation formula where $f(x)=x^3+2$ and $x=$ 0, 1, 2, 3, 4, 5.

**Solution:**

| $x$ | $f(x)$ | $\Delta$ | $\Delta^2$ | $\Delta^3$ | $\Delta^4$ |
|---|---|---|---|---|---|
| 0 | 2 | | | | |
| | | 1 | | | |
| 1 | 3 | | 6 | | |
| | | 7 | | | |
| 2 | 10 | | 12 | | |
| | | 19 | | 6 | |
| 3 | 29 | | 18 | | 0 |

| | | | | | | |
|---|---|---|---|---|---|---|
| | | 37 | | 6 | | |
| 4 | 66 | | 24 | | | |
| | | 61 | | | | |
| 5 | 127 | | | | | |

If $x$=2.31, $h$=1$\Rightarrow$ $s=\dfrac{x-x_0}{h}=\dfrac{2.31-2}{1}=0.31$ .

$$p_3(x)=y_0+s\Delta y_0+\frac{s(s-1)}{2!}\Delta^2 y_0+\frac{s(s-1)(s-2)}{3!}\Delta^3 y_0 .$$

Hence

$$p_3'(x)=\frac{1}{h}\left\{\Delta y_0+(s-\frac{1}{2})\Delta^2 y_0+(\frac{s^2}{2}-s+\frac{1}{3})\Delta^3 y_0\right\}$$

and

$$f'(2.31)\cong p_3'(2.31)=19+(0.31-0.5)(18)+(\frac{(0.31)^2}{2}-0.31+\frac{1}{3})(6)=16.008 \quad .$$

To find the exact value of $f'(x)$ differentiate $f(x)$ directly with respect to $x$ , we get

$$f'(x)=3x^2 \Rightarrow f'(2.31)=3(2.31)^2=16.0083 \quad (\text{exact value}) .$$

Error=exact value-approximate value=16.0083-16.008=0.0003.

If $x$=1, $h$=1$\Rightarrow$ $s=\dfrac{x-x_0}{h}=\dfrac{1-1}{1}=0$ .

$$p_3(x)=y_0+s\Delta y_0+\frac{s(s-1)}{2!}\Delta^2 y_0+\frac{s(s-1)(s-2)}{3!}\Delta^3 y_0 \Rightarrow p_3'(x)=\frac{1}{h}\left\{\Delta y_0+(s-\frac{1}{2})\Delta^2 y_0+(\frac{s^2}{2}-s+\frac{1}{3})\Delta^3 y_0\right\}$$

$$p_3'(x)=\frac{1}{h}\left\{\Delta y_0-\frac{1}{2}\Delta^2 y_0+\frac{1}{3}\Delta^3 y_0\right\}$$

$$\therefore\ f'(1)\cong p_3'(1)=7-\frac{1}{2}(12)+\frac{1}{3}(6)=3$$

$$f'(x)=3x^2 \Rightarrow f'(1)=3(1)^2=3 \ (\text{exact value})$$

Error=exact value-approximate value=3-3=0.

**Theorem 7.1:** Let $f(x)$ is continuously differentiable ($n$+1) times on [a,b], then

$$f'(x_j)-p_n'(x_j)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{\substack{i=0\\ i\neq j}}^{n}(x_j-x_i)\ ,\ j=0,\ 1,\ \ldots,\ n.$$

**Proof:** From errors in interpolation, we have

$$f(x)-p_n(x)=\frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{i=0}^{n}(x-x_i) .$$

Let $g(x) = \dfrac{f^{(n+1)}(\xi)}{(n+1)!}$ and $w(x) = \prod_{i=0}^{n}(x - x_i) \Rightarrow f(x) - p_n(x) = g(x)w(x)$.

$\therefore f'(x) - p'_n(x) = g(x)w'(x) + g'(x)w(x) \Rightarrow f'(x_j) - p'_n(x_j) = g(x_j)w'(x_j) + g'(x_j)w(x_j)$, but

$w(x_j) = 0$, for $j = 0, 1, 2, \ldots, n$.

$\therefore f'(x_j) - p'_n(x_j) = g(x_j)w'(x_j)$.

$$w'(x_j) = \prod_{\substack{i=0 \\ i \neq j}}^{n}(x_j - x_i)$$

$$\therefore f'(x_j) - p'_n(x_j) = \frac{f^{(n+1)}(\xi)}{(n+1)!}\prod_{\substack{i=0 \\ i \neq j}}^{n}(x_j - x_i).$$

We can use **forward difference** for discrete functions as follows:

We know

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

For a finite $\Delta x$,

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

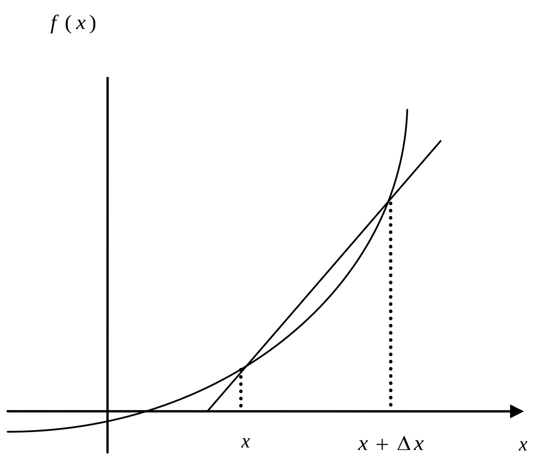


**Figure 7.3.** Graphical representation of forward difference approximation of first derivative.

So given $n+1$ data points $(x_0, y_0), (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$, the value of $f'(x)$ for $x_i \leq x \leq x_{i+1}$, $i = 0, \ldots, n-1$, is given by

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

**Example 7.8:** The upward velocity of a rocket is given as a function of time in Table 7.3.

**Table 7.3** Velocity as a function of time.

| $t$ (s) | $v(t)$ (m/s) |
|---|---|
| 0 | 0 |
| 10 | 227.04 |
| 15 | 362.78 |
| 20 | 517.35 |
| 22.5 | 602.97 |
| 30 | 901.67 |

Using forward divided difference, find the acceleration of the rocket at $t = 16$ s .

**Solution:** To find the acceleration at $t = 16$ s , we need to choose the two values of velocity closest to $t = 16$ s , that also bracket $t = 16$ s to evaluate it. The two points are $t = 15$ s and $t = 20$ s

$$a(t_i) \approx \frac{v(t_{i+1}) - v(t_i)}{\Delta t}, \; t_i = 15, \; t_{i+1} = 20, \; \Delta t = t_{i+1} - t_i = 20 - 15 = 5,$$

$$a(16) \approx \frac{v(20) - v(15)}{5} = \frac{517.35 - 362.78}{5}$$

$$= 30.914 \text{ m/s}^2 .$$