Chapter 5 Numerical Differentiation and Integration

1. Numerical Differentiation

Taylor's expansion

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

$$where \qquad f'(x_i) = \frac{df}{dx} \qquad at \qquad (x = x_i)$$

First Derivatives

Let

$$h = \Delta x = (x_i - x_{i-1}) \qquad and \qquad is \qquad small$$

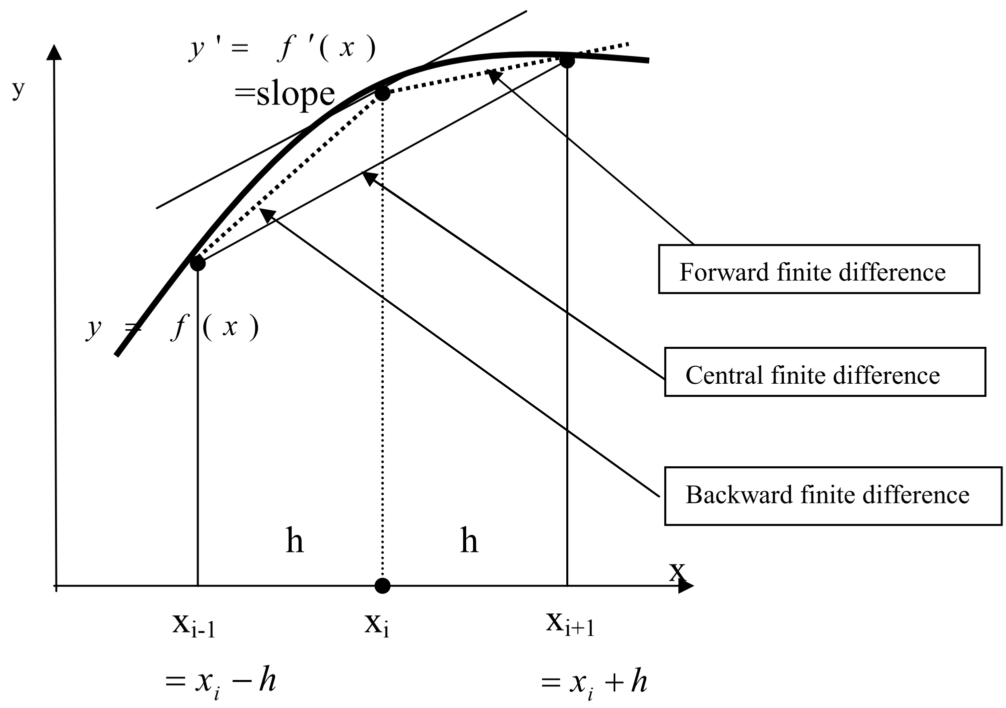


Figure 1. Numerical differentiation based on Taylor'series

Forward finite difference

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

or

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

Backward finite difference

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

or

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

The error is $E_1 \propto h$, with the order of O(h) or which is proportional to h.

and

Central finite difference

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{h^2 f'''(x_i)}{6} + \ldots$$

or

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + \text{error}$$

The error is $\boldsymbol{E}_1 \propto \boldsymbol{h}^2$, with the order of $O(h^2)$ or which is proportional to h^2.

Second Derivatives

Expansions of Taylor's series for $f(x_{i+2})$ (with $x - x_i = 2\Delta x = 2h$)

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

and also

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

Subtracting the two equations giving

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

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

$$\boldsymbol{f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2}} \qquad \textbf{\textit{forward} – \textit{difference}}$$

The error is $\boldsymbol{E_2 \propto \Delta x}$, with the order of O(Δx)

Similarly, expansions of Taylor's series for $f(x_{i-2})$ (with $x - x_i = -2\Delta x = -2h$) giving

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

$$\boldsymbol{f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{(\Delta x)^2}} \qquad \textbf{\textit{backward} – \textit{difference}}$$

In additions

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

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

Giving

$$\boldsymbol{f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(\Delta x)^2} - \frac{(\Delta x)^2}{12} f''''(x_i) +}$$

$$\boldsymbol{f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(\Delta x)^2}} \qquad \textbf{\textit{central -- difference}}$$

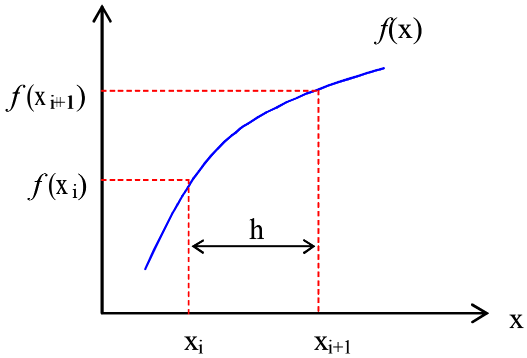
The error is $\boldsymbol{E}_2 \propto (\Delta \boldsymbol{x})^2$, with the order of $O(\Delta x)^2$

Example 1:

Assume time t and displacement f(t) are known. Calculate the velocity f'(t) and acceleration f″ (t).

i	Time t_i	Displacement y_i=f(t_i)	h=Δt	$\boxed{f'(t)}$	$\boxed{f''(t)}$
1	0.05	0.144	0.05	0.56	
2	0.1	0.172	0.05		
3	0.15	0.213	0.05		
4	0.2	0.296	0.05	-1.43	-123.6
5	0.25	0.07	0.05		
6	0.3	0.085	0.05		
7	0.35	0.525	0.05		
8	0.4	0.11	0.05		
9	0.45	0.062	0.05		
10	0.5	0.055	0.05		
11	0.55	0.042	0.05		
12	0.6	0.035	0.05	-0.14	

Solution



Forward Difference

$$\boxed{f'(t_i) = \frac{f(t_{i+1}) - f(t_i)}{\Delta t}}$$

$$\boxed{f''(t_i) = \frac{f(t_{i+2}) - 2f(t_{i+1}) + f(t_i)}{(\Delta t)^2}}$$

Central Difference

$$\boxed{f'(t_i) = \frac{f(t_{i+1}) - f(t_{i-1})}{2\Delta t}}$$

$$\boxed{f''(t_i) = \frac{f(t_{i+1}) - 2f(t_i) + f(t_{i-1})}{(\Delta t)^2}}$$

Backward Difference

$$\boxed{f'(t_i) = \frac{f(t_i) - f(t_{i-1})}{\Delta t}}$$

$$\boxed{f''(t_i) = \frac{f(t_i) - 2f(t_{i-1}) + f(t_{i-2})}{(\Delta t)^2}}$$

Example 2:

Compare the results of numerical differentiation and the exact solution on the following function f(x)=cos(x) at $x = \pi/6$, with different intervals h chosen.

Solution

At $x_i = \pi/6$ for different h between $0.00001 < h < 0.1$.

(1) Using Forward Finite Difference

$$f(x_i) = \cos(x_i)$$

$$f'(x_i) = -\sin(x_i) \quad is \quad exact$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} = \frac{\cos(x_i + h) - \cos(x_i)}{h} \quad is \quad numerical$$

h	x_i=	$f'(x_i)$	$f'(x_i)$	error	% error
	$\pi/6$	*exact*	numerical		
0.1	0.523599	-0.5	-0.54243228	-0.04243228	8.486456%
0.01	0.523599	-0.5	-0.50432176	-0.00432176	0.864352%
0.001	0.523599	-0.5	-0.50043293	-0.00043293	0.086586%
0.0001	0.523599	-0.5	-0.50004330	-0.00004330	0.008660%
0.00001	0.523599	-0.5	-0.50000433	-0.00000433	0.000866%

(2) Using Central Finite Difference

$$f(x_i) = \cos(x_i)$$

$$f'(x_i) = -\sin(x_i) \quad is \quad exact$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} = \frac{\cos(x_i + h) - \cos(x_i - h)}{2h} \quad is \quad numerical$$

h	x_i=	$f'(x_i)$	$f'(x_i)$	error	% error
	$\pi/6$	*exact*	numerical		
0.1	0.523599	-0.5	-0.49916708	0.00083292	-0.166583%
0.01	0.523599	-0.5	-0.49999167	0.00000833	-0.001667%
0.001	0.523599	-0.5	-0.49999992	0.00000008	-0.000017%
0.0001	0.523599	-0.5	-0.50000000	0.00000000	0.000000%

Example 3: Numerically calculate $\frac{\partial^2 T(x,t)}{\partial^2 x}$ at t=0.02 based on the table of T(x,t) at different times t and positions x, as follows.

	x_1=0	x_2=0.2	x_3=0.4	x_4=0.6	x_5=0.8	x_6=1.0
t=0	0.0	0.64	0.96	0.96	0.64	0.0
t=0.02	0.0	0.48	0.80	0.80	0.48	0.0

Ans:

Using the central difference scheme for second derivative and Δ x=0.2, we have

$$\frac{\partial^2 T(x,t)}{\partial^2 x}\Big|_{t\ \ fixed;\quad x=x_i} = \frac{T(x_{i+1},t) - 2T(x_i,t) + T(x_{i-1},t)}{(\Delta x)^2}$$

at x_2 to x_5 and at time t=0.02, as follows.

	x_1=0	x_2=0.2	x_3=0.4	x_4=0.6	x_5=0.8	x_6=1.0
t=0.02		-4	-8	-8	-4	

Example 4: The temperatures of a thin rod are tabulated below. The temperature *T(x,t)* is in unit of °C; the positions x_1 to x_6 are in unit of *cm*; time *t* is in unit of second.

	x_1=0	x_2=0.2	x_3=0.4	x_4=0.6	x_5=0.8	x_6=1.0
t=0	0.0	64	96	96	64	0.0
t=0.02	0.0	48	80	80	48	0.0
t=0.04	0.0	40	64	64	40	0.0

Verify by calculating $\partial T / \partial t$ using the forward finite difference and $\partial^2 T / \partial x^2$ using the central finite difference that the temperatures *T(x,t)* listed in the table are solutions to the heat conduction equation $\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$ at x_2 to x_5 and at time t=0.02 s.

Ans:

Using forward finite difference:

$$\partial T / \partial t \approx [T(x, t+\Delta t) - T(x,t)] / \Delta t$$

At position $x=x_i$ ($i=3$) and $t=0.02$ with $\Delta t=0.02$:

$$\frac{\partial T}{\partial t}\Big|_{x=x_i} \approx [T(x_i, t+0.02) - T(x_i, t)] / 0.02$$

Thus $\partial T / \partial t$ is

	$x_3=0.4$
t=0.02	-800

Using center finite difference:

$$\partial^2 T / \partial x^2 \approx [T(x+\Delta x, t) - 2T(x,t) + T(x-\Delta x, t)] / (\Delta x)^2$$

At point i=3:

$$\frac{\partial^2 T}{\partial x^2}\Big|_{t=0.02} \approx [T(x_{i+1}, t) - 2T(x_i, t) + T(x_{i-1}, t)] / (\Delta x)^2$$

Thus $\partial^2 T / \partial x^2$ at $x=x_i$ and $t=0.02$ with $\Delta x=0.2$ is

	$x_3=0.4$
t=0.02	-800

Therefore the temperature at t=0.02 and $x=x_3=0.4$ *cm* listed in the table satisfies the equation $\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$

Similarly,

at position $x=x_i$ ($i=4$) and $t=0.02$ the equation is

$$\frac{\partial T}{\partial t} = -800 = \frac{\partial^2 T}{\partial x^2} \ ;$$

at position $x=x_i$ ($i=2$ and 5) and $t=0.02$ the equation is

$$\frac{\partial T}{\partial t} = -400 = \frac{\partial^2 T}{\partial x^2}$$

2. Numerical Integration

Newton-Cotes formulas for integration

$$I = \int_a^b f(x)dx \cong \int_a^b f_n(x)dx$$

$$where \quad f_n(x) \quad is \quad polynomial$$

$$f_n(x) = a_0 + a_1 x + \cdots + a_{n-1}x^{n-1} + a_n x^n$$

Trapezoidal Rule

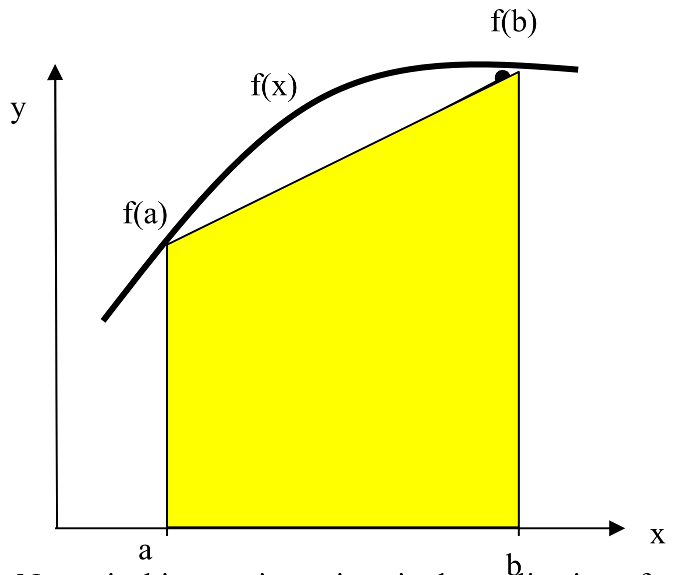


Figure 2. Numerical integration using single-application of trapezoidal rule

By Newton-Cotes formula

$$I = \int_a^b f(x)dx \cong \int_a^b f_1(x)dx$$

$$where \quad f_1(x) \quad is \quad a\ polynomial$$

$$f_1(x) = a_0 + a_1(x-a) = f(a) + \frac{f(b)-f(a)}{b-a}(x-a)$$

$$I = \int_a^b f_1(x)dx = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx$$

Integrating

$$I = \int_a^b f_1(x)dx = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx = (b - a)\frac{f(a) + f(b)}{2}$$

Example 5:

Calculate $I = \int_a^b f(x)dx$ using trapezoidal rule, where

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

$a = 0.0;\qquad b = 0.8$

$f(0) = 0.2$

$f(0.8) = 0.232$

$I_{exact} = 1.640533$

<u>Solution</u>

$$I = (b - a)\frac{f(a) + f(b)}{2} = (0.8)\left(\frac{0.2 + 0.232}{2}\right) = 0.1728$$

$$Error \quad = \quad 1.640533 - 0.1728 = 1.467733 \qquad or \qquad 89.5\%$$

Multiple-application of trapezoidal rule

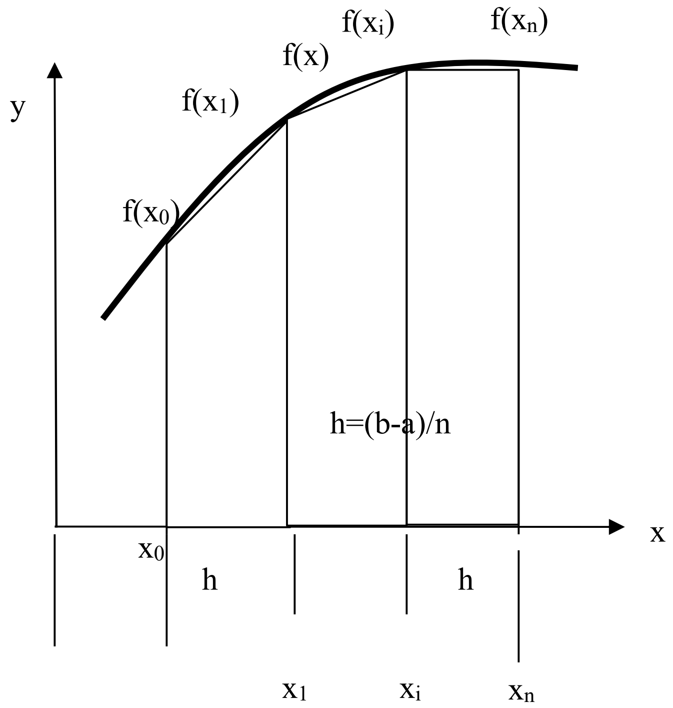


Figure 3. Numerical integration using multiple-application of trapezoidal rule

Because

$$h = \frac{(b-a)}{n}$$

Hence

$$I = \int_{x_0}^{x_1} f\,(x)dx + \int_{x_1}^{x_2} f\,(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f\,(x)dx$$

$$= h\left(\frac{f(x_0)+f(x_1)}{2}\right) + h\left(\frac{f(x_1)+f(x_2)}{2}\right) + \cdots + h\left(\frac{f(x_{n-1})+f(x_n)}{2}\right)$$

$$= \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

Example 6：

Calculate $I = \int_a^b f(x)\,dx$ using trapezoidal rule, where

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

$a = 0.0;\qquad b = 0.8$

$n = 2;\qquad h = 0.4$

$f(0) = 0.2$

$f(0.4) = 2.456$

$f(0.8) = 0.232$

$I_{exact} = 1.640533$

<u>Solution</u>

$$I = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n) \right]$$

$$= \frac{0.4}{2}\left[0.2 + 2(2.456) + 0.232\right] = 1.0688 \qquad with \quad error = 34.9\%$$

Simpson's 1/3 Rule

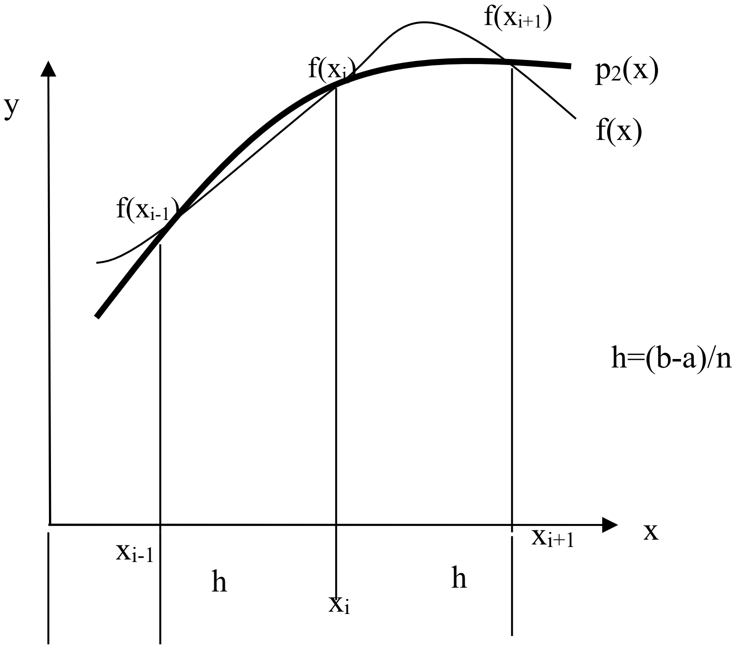


Figure 4. Numerical integration using using single-application of Simpson's 1/3 rule

$$I = \int_a^b f(x)dx \cong \int_{x_{i-1}}^{x_{i+1}} p_2(x)dx$$

where $p_2(x)$ *is a parabola*

$p_2(x) = c_0 + c_1 x + c_2 x^2$ passing (x_{i-1}, f_{i-1}); (x_i, f_i); (x_{i+1}, f_{i+1})

Taking origin at x_i with x_{i-1}=-h and x_{i+1}=h,

$$p_2(-h) = f_{i-1} = c_0 + c_1(-h) + c_2(-h)^2 = c_0 - c_1(h) + c_2(h)^2$$
$$p_2(0) = f_i = c_0 + c_1(0) + c_2(0)^2 = c_0$$
$$p_2(h) = f_{i+1} = c_0 + c_1(h) + c_2(h)^2$$

giving

$$c_0 = f_i; \quad c_1 = \frac{f_{i+1} - f_{i-1}}{2h} \quad ; \quad c_2 = \frac{f_{i-1} - 2f_i + f_{i+1}}{2h^2}$$

$$I = \int_a^b f(x)dx \cong \int_{x_{i-1}}^{x_{i+1}} p_2(x)dx$$

where $\quad p_2(x) = c_0 + c_1 x + c_2 x^2$

$$I = \int_{-h}^{h} \left(c_0 + c_1 x + c_2 x^2\right)dx = c_0 x + \frac{c_1}{2}x^2 + \frac{c_2}{3}x^3 \Big|_{-h}^{h} = \frac{2c_2}{3}h^3 + 2c_0 h$$

$$= \frac{h}{3}\left(f_{i-1} + 4f_i + f_{i+1}\right)$$

Multiple application of Simpson’s rule gives

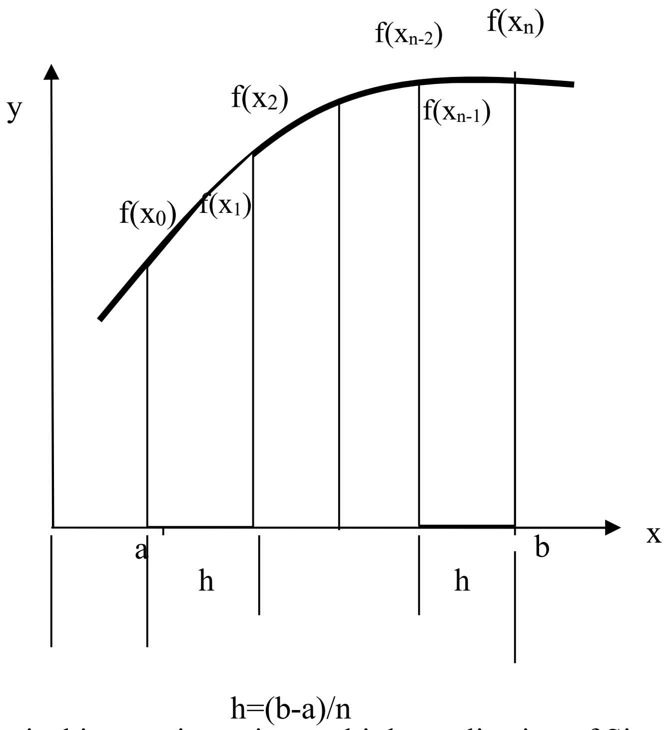


Figure 5. Numerical integration using multiple-application of Simpson’s 1/3 rule

Taking $\quad h = \dfrac{b-a}{n}$

$$I = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)dx$$

$$= 2h\left(\frac{f(x_0)+4f(x_1)+f(x_2)}{6}\right) + 2h\left(\frac{f(x_2)+4f(x_3)+f(x_4)}{6}\right) + \cdots$$
$$+ 2h\left(\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}\right)$$

$$I = \int_a^b f(x)dx = \frac{h}{3}(f_0 + 4\sum_{i=1,3,5,\ldots}^{n-1} f_i + 2\sum_{i=2,4,6,\ldots}^{n-2} f_i + f_n)$$

Example 7:

Calculate $I = \int_a^b f(x)dx$ using Simpson's 1/3 rule with a=0, b=0.8 and h = 0.4

$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$

$I_{exact} = 1.640533$

<u>Solution</u>

$$I = \int_0^{0.8} f(x)dx$$
$$= \frac{h}{3}[f(0) + 4f(0.4) + f(0.8)]$$
$$= 1.367466$$

Error=16.6%