NUMERICAL DIFFERENTIATION

The derivative of *f (x)* at x_0 is:

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

An approximation to this is:

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h}$$

for small values of *h*.

Forward Difference Formula

Let $f(x) = \ln x$ and $x_0 = 1.8$

Find an approximate value for $f'(1.8)$

h	$f(1.8)$	$f(1.8+h)$	$\dfrac{f(1.8+h)-f(1.8)}{h}$
0.1	0.5877867	0.6418539	0.5406720
0.01	0.5877867	0.5933268	0.5540100
0.001	0.5877867	0.5883421	0.5554000

The exact value of $f'(1.8) = 0.55\overline{5}$

Assume that a function goes through three points:

$$\left(x_0, f\left(x_0\right)\right), \left(x_1, f\left(x_1\right)\right) \textbf{ and } \left(x_2, f\left(x_2\right)\right).$$

$$f(x) \approx P(x)$$

$$P(x) = L_0(x) f(x_0) + L_1(x) f(x_1) + L_2(x) f(x_2)$$

Lagrange Interpolating Polynomial

$$P(x) = L_0(x) f(x_0) + L_1(x) f(x_1) + L_2(x) f(x_2)$$

$$P(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0)$$

$$+ \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1)$$

$$+ \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

$$f'(x) \approx P'(x)$$

$$P'(x) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f(x_0)$$

$$+ \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} f(x_1)$$

$$+ \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

If the points are equally spaced, i.e.,

$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h$$

$$P'(x_0) = \frac{2x_0 - (x_0 + h) - (x_0 + 2h)}{\{x_0 - (x_0 + h)\}\{x_0 - (x_0 + 2h)\}} f(x_0)$$

$$+ \frac{2x_0 - x_0 - (x_0 + 2h)}{\{(x_0 + h) - x_0\}\{(x_0 + h) - (x_0 + 2h)\}} f(x_1)$$

$$+ \frac{2x_0 - x_0 - (x_0 + h)}{\{(x_0 + 2h) - x_0\}\{(x_0 + 2h) - (x_0 + h)\}} f(x_2)$$

$$P'(x_0) = \frac{-3h}{2h^2} f(x_0) + \frac{-2h}{-h^2} f(x_1) + \frac{-h}{2h^2} f(x_2)$$

$$P'(x_0) = \frac{1}{2h}\left\{-3f(x_0) + 4f(x_1) - f(x_2)\right\}$$

Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\left\{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right\}$$

If the points are equally spaced with x_0 in the middle:

$$x_1 = x_0 - h \text{ and } x_2 = x_0 + h$$

$$P'(x_0) = \frac{2x_0 - (x_0 - h) - (x_0 + h)}{\{x_0 - (x_0 - h)\}\{(x_0 - (x_0 + h)\}} f(x_0)$$

$$+ \frac{2x_0 - x_0 - (x_0 + h)}{\{(x_0 - h) - x_0\}\{(x_0 - h) - (x_0 + h)\}} f(x_1)$$

$$+ \frac{2x_0 - x_0 - (x_0 - h)}{\{(x_0 + h) - x_0\}\{(x_0 + h) - (x_0 - h)\}} f(x_2)$$

$$P'(x_0) = \frac{0}{-h^2} f(x_0) + \frac{-h}{2h^2} f(x_1) + \frac{h}{2h^2} f(x_2)$$

Another Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{f(x_0+h) - f(x_0-h)\}$$

Alternate approach (Error estimate)

Take Taylor series expansion of $f(x+h)$ about x:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f^{(2)}(x) + \frac{h^3}{3!} f^{(3)}(x) + \cdots$$

$$f(x+h) - f(x) = hf'(x) + \frac{h^2}{2} f^{(2)}(x) + \frac{h^3}{3!} f^{(3)}(x) + \cdots$$

$$\frac{f(x+h) - f(x)}{h} = f'(x) + \frac{h}{2} f^{(2)}(x) + \frac{h^2}{3!} f^{(3)}(x) + \cdots$$

.... (1)

$$\frac{f(x+h)-f(x)}{h} = f'(x) + O(h)$$

$$f'(x) = \frac{f(x+h)-f(x)}{h} - O(h)$$

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

Forward Difference Formula

$$O(h) = \frac{h}{2} f^{(2)}(x) + \frac{h^2}{3!} f^{(3)}(x) + \cdots$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{4h^2}{2} f^{(2)}(x) + \frac{8h^3}{3!} f^{(3)}(x) + \cdots$$

$$f(x+2h) - f(x) = 2hf'(x) + \frac{4h^2}{2} f^{(2)}(x) + \frac{8h^3}{3!} f^{(3)}(x) + \cdots$$

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

.... (2)

$$\frac{f(x+h)-f(x)}{h}=f'(x)+\frac{h}{2}f^{(2)}(x)+\frac{h^2}{3!}f^{(3)}(x)+\cdots$$

…………… (1)

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

……………… (2)

2 X Eqn. (1) – Eqn. (2)

$$2\frac{f(x+h)-f(x)}{h}-\frac{f(x+2h)-f(x)}{2h}$$

$$=f'(x)-\frac{2h^2}{3!}f^{(3)}(x)-\frac{6h^3}{4!}f^{(4)}(x)-\cdots$$

$$\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}$$

$$=f'(x)-\frac{2h^2}{3!}f^{(3)}(x)-\frac{6h^3}{4!}f^{(4)}(x)-\cdots$$

$$=f'(x)+O(h^2)$$

$$\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h} = f'(x)+O(h^2)$$

$$f'(x) = \frac{-f(x+2h)+4f(x+h)-3f(x)}{2h} - O(h^2)$$

$$f'(x) \approx \frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}$$

Three-point Formula

$$O(h^2) = -\frac{2h^2}{3!} f^{(3)}(x) - \frac{6h^3}{4!} f^{(4)}(x) - \cdots$$

The Second Three-point Formula

Take Taylor series expansion of *f*(*x*+*h*) about *x*:

$$f\left(x+h\right)=f\left(x\right)+hf'\left(x\right)+\frac{h^2}{2}f^{(2)}\left(x\right)+\frac{h^3}{3!}f^{(3)}\left(x\right)+\cdots$$

Take Taylor series expansion of *f*(*x*-*h*) about *x*:

$$f\left(x-h\right)=f\left(x\right)-hf'\left(x\right)+\frac{h^2}{2}f^{(2)}\left(x\right)-\frac{h^3}{3!}f^{(3)}\left(x\right)+\cdots$$

Subtract one expression from another

$$f\left(x+h\right)-f\left(x-h\right)=2hf'\left(x\right)+\frac{2h^3}{3!}f^{(3)}\left(x\right)+\frac{2h^6}{6!}f^{(6)}\left(x\right)+\cdots$$

$$f(x+h)-f(x-h)=2hf'(x)+\frac{2h^3}{3!}f^{(3)}(x)+\frac{2h^6}{6!}f^{(6)}(x)+\cdots$$

$$\frac{f(x+h)-f(x-h)}{2h}=f'(x)+\frac{h^2}{3!}f^{(3)}(x)+\frac{h^5}{6!}f^{(6)}(x)+\cdots$$

$$f'(x)=\frac{f(x+h)-f(x-h)}{2h}-\frac{h^2}{3!}f^{(3)}(x)-\frac{h^5}{6!}f^{(6)}(x)-\cdots$$

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

$$O(h^2) = -\frac{h^2}{3!} f^{(3)}(x) - \frac{h^5}{6!} f^{(6)}(x) - \cdots$$

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

Second Three-point Formula

Summary of Errors

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

Forward Difference Formula

Error term $$O(h) = \frac{h}{2} f^{(2)}(x) + \frac{h^2}{3!} f^{(3)}(x) + \cdots$$

Summary of Errors continued

First Three-point Formula

$$f'(x) \approx \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h}$$

Error term $O(h^2) = -\frac{2h^2}{3!} f^{(3)}(x) - \frac{6h^3}{4!} f^{(4)}(x) - \cdots$

Summary of Errors continued

Second Three-point Formula

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

Error term $O\left(h^2\right) = -\frac{h^2}{3!} f^{(3)}(x) - \frac{h^5}{6!} f^{(6)}(x) - \cdots$

Example:

$$f(x) = xe^x$$

Find the approximate value of $f'(2)$ **with** $h = 0.1$

x	$f(x)$
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Using the Forward Difference formula:

$$f'(x_0) \approx \frac{1}{h}\left\{f(x_0+h)-f(x_0)\right\}$$

$$f'(2) \approx \frac{1}{0.1}\left\{f(2.1)-f(2)\right\}$$

$$= \frac{1}{0.1}\left\{17.148957-14.778112\right\}$$

$$= 23.708450$$

Using the 1st Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\left\{-3f(x_0)+4f(x_0+h)-f(x_0+2h)\right\}$$

$$f'(2) \approx \frac{1}{2\times 0.1}\left[-3f(2)+4f(2.1)-f(2.2)\right]$$

$$= \frac{1}{0.2}\left[-3\times 14.778112+4\times 17.148957 -19.855030\right]$$

$$= 22.032310$$

Using the 2nd Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{f(x_0+h) - f(x_0-h)\}$$

$$f'(2) \approx \frac{1}{2\times 0.1}\left[f(2.1) - f(1.9)\right]$$

$$= \frac{1}{0.2}\left[17.148957 - 12.703199\right]$$

$$= 22.228790$$

The exact value of $f'(2)$ is : 22.167168

Comparison of the results with $h = 0.1$

The exact value of $f'(2)$ is 22.167168

Formula	$f'(2)$	Error
Forward Difference	23.708450	1.541282
1st Three-point	22.032310	0.134858
2nd Three-point	22.228790	0.061622

Second-order Derivative

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f^{(2)}(x) + \frac{h^3}{3!} f^{(3)}(x) + \cdots$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f^{(2)}(x) - \frac{h^3}{3!} f^{(3)}(x) + \cdots$$

Add these two equations.

$$f(x+h) + f(x-h) = 2f(x) + \frac{2h^2}{2} f^{(2)}(x) + \frac{2h^4}{4!} f^{(4)}(x) + \cdots$$

$$f(x+h) - 2f(x) + f(x-h) = \frac{2h^2}{2} f^{(2)}(x) + \frac{2h^4}{4!} f^{(4)}(x) + \cdots$$

$$\frac{f(x+h)-2f(x)+f(x-h)}{h^2}=f^{(2)}(x)+\frac{2h^2}{4!}f^{(4)}(x)+\cdots$$

$$f^{(2)}(x)=\frac{f(x+h)-2f(x)+f(x-h)}{h^2}-\frac{2h^2}{4!}f^{(4)}(x)+\cdots$$

$$f^{(2)}(x)\approx\frac{f(x+h)-2f(x)+f(x-h)}{h^2}$$

Newton Forward difference Polynomial

$$P_n(x)$$

$$= f_0 + s\nabla f_0 + \frac{s(s-1)}{2!}\nabla^2 f_0 + \cdots$$

$$+ \frac{s(s-1)(s-2)\ldots(s-n+1)}{n!}\nabla^n f_0$$

$$x = x_0 + sh \quad \Longrightarrow \quad s = \frac{x - x_0}{h}$$

$$\frac{dP_n(x)}{dx} = \frac{dP_n(x)}{ds}\frac{ds}{dx}$$

$$\frac{dP_n(x)}{ds} = \Delta f_0 + \frac{2s-1}{2}\Delta^2 f_0 + \frac{3s^2-6s+2}{6}\Delta^3 f_0 + ...$$

$$\frac{dx}{ds} = h$$

$$\frac{dP_n(x)}{dx} = \frac{1}{h}\left[\begin{array}{l} \Delta f_0 + \dfrac{2s-1}{2}\Delta^2 f_0 + \dfrac{3s^2-6s+2}{6}\Delta^3 f_0 + \\ \dfrac{4s^3-18s^2+22s-6}{24}\Delta^4 f_0 + ... \end{array}\right]$$

Newton backward difference Polynomial

$$P_b(x) = f_0 + s\nabla f_0 + \frac{s(s+1)}{2!}\nabla^2 f_0 + \cdots$$
$$+ \frac{s(s+1)\ldots(s+n-1)}{n!}\frac{\nabla^n f_0}{n!}$$

$$\frac{dP_b(x)}{dx} = \frac{1}{h}\left[\begin{array}{l} \Delta f_0 + \dfrac{2s+1}{2}\Delta^2 f_0 + \dfrac{3s^2+6s+2}{6}\Delta^3 f_0 + \\ \dfrac{4s^3+18s^2+22s+6}{24}\Delta^4 f + \ldots. \end{array}\right]$$

Compute $f'(0.2)$ from the following tabular data.

x	0.0	0.2	0.4	0.6	0.8	1.0
$f(x)$	1.00	1.16	3.56	13.96	41.96	101.00

Compute $f'(0.2)$ from the following tabular data.

x	0.0	0.2	0.4	0.6	0.8	1.0
$f(x)$	1.00	1.16	3.56	13.96	41.96	101.00

x	$y=f(x)$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
0.0	1.00					
		0.16				
0.2	1.16		2.24			
		2.40		5.76		
0.4	3.56		8.00		3.84	
		10.40		9.60		0.00
0.6	13.96		17.60		3.84	
		28.00		13.44		
0.8	41.96		31.04			
		59.04				
1.0	101.00					

x	$y=f(x)$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
0.0	1.00					
		0.16				
0.2	1.16		2.24			
		2.40		5.76		
0.4	3.56		8.00		3.84	
		10.40		9.60		0.00
0.6	13.96		17.60		3.84	
		28.00		13.44		
0.8	41.96		31.04			
		59.04				
1.0	101.00					

$$\frac{dP_n(x)}{dx} = \frac{1}{h}\left[\Delta f_0 + \frac{2s-1}{2}\Delta^2 f_0 + \frac{3s^2-6s+2}{6}\Delta^3 f_0 + \frac{4s^3-18s^2+22s-6}{24}\Delta^4 f_0 + \ldots\ldots\right]$$

x	$y=f(x)$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
0.0	1.00					
		0.16				
0.2	1.16		2.24			
		2.40		5.76		
0.4	3.56		8.00		3.84	
		10.40		9.60		0.00
0.6	13.96		17.60		3.84	
		28.00		13.44		
0.8	41.96		31.04			
		59.04				
1.0	101.00					

$$S = \frac{(0.2-0.0)}{0.2} = 1$$

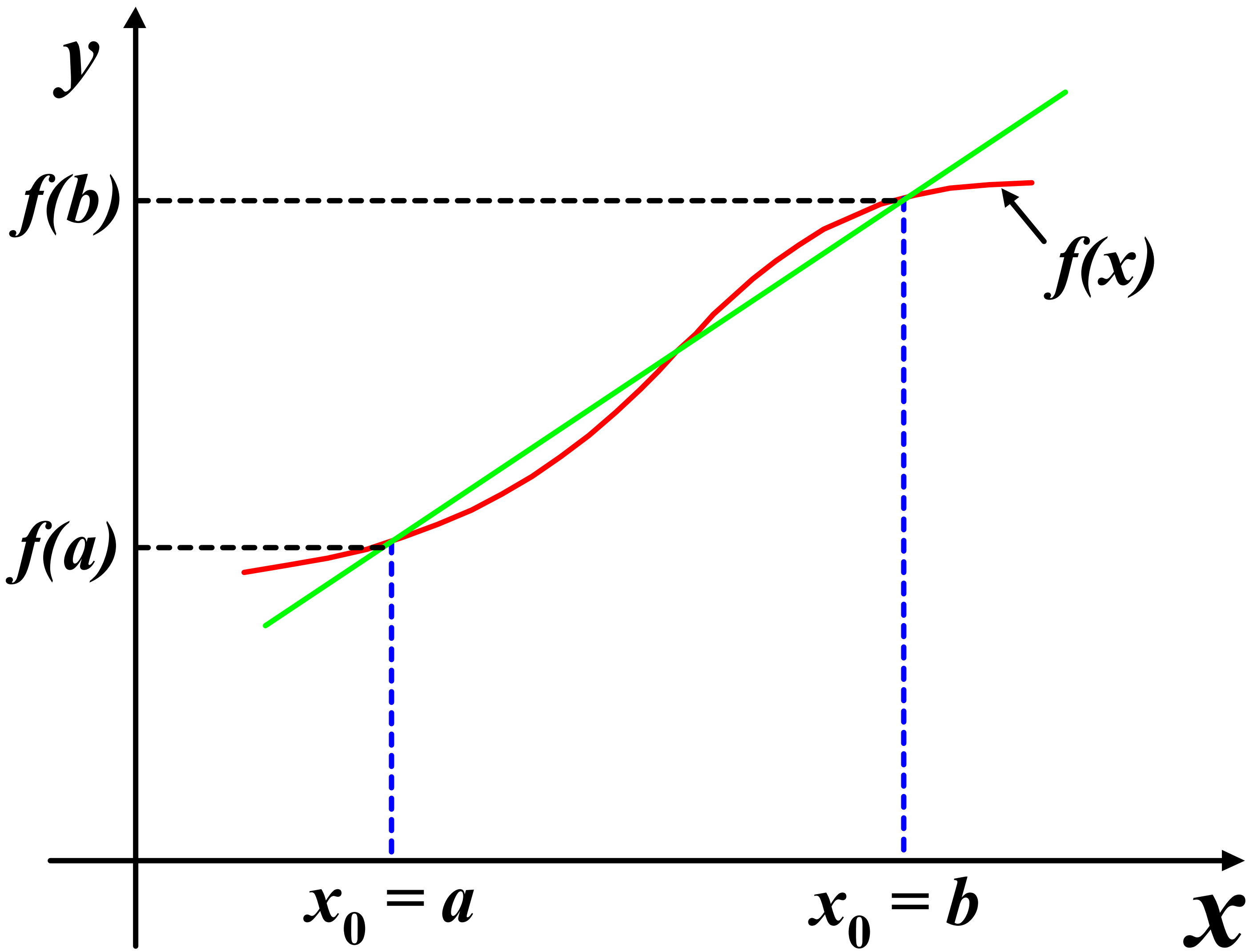
$$\left.\frac{d}{dx} f(x)\right|_{x=0.2} = \frac{1}{0.2}\left[0.16 + \frac{2\times 1 - 1}{2!}[2.24] + \frac{3\times 1^2 - 6\times 1 + 2}{3!}[5.76] + \frac{4\times 1^3 - 18\times 1^2 + 22\times 1 - 6}{24}[3.84]\right]$$

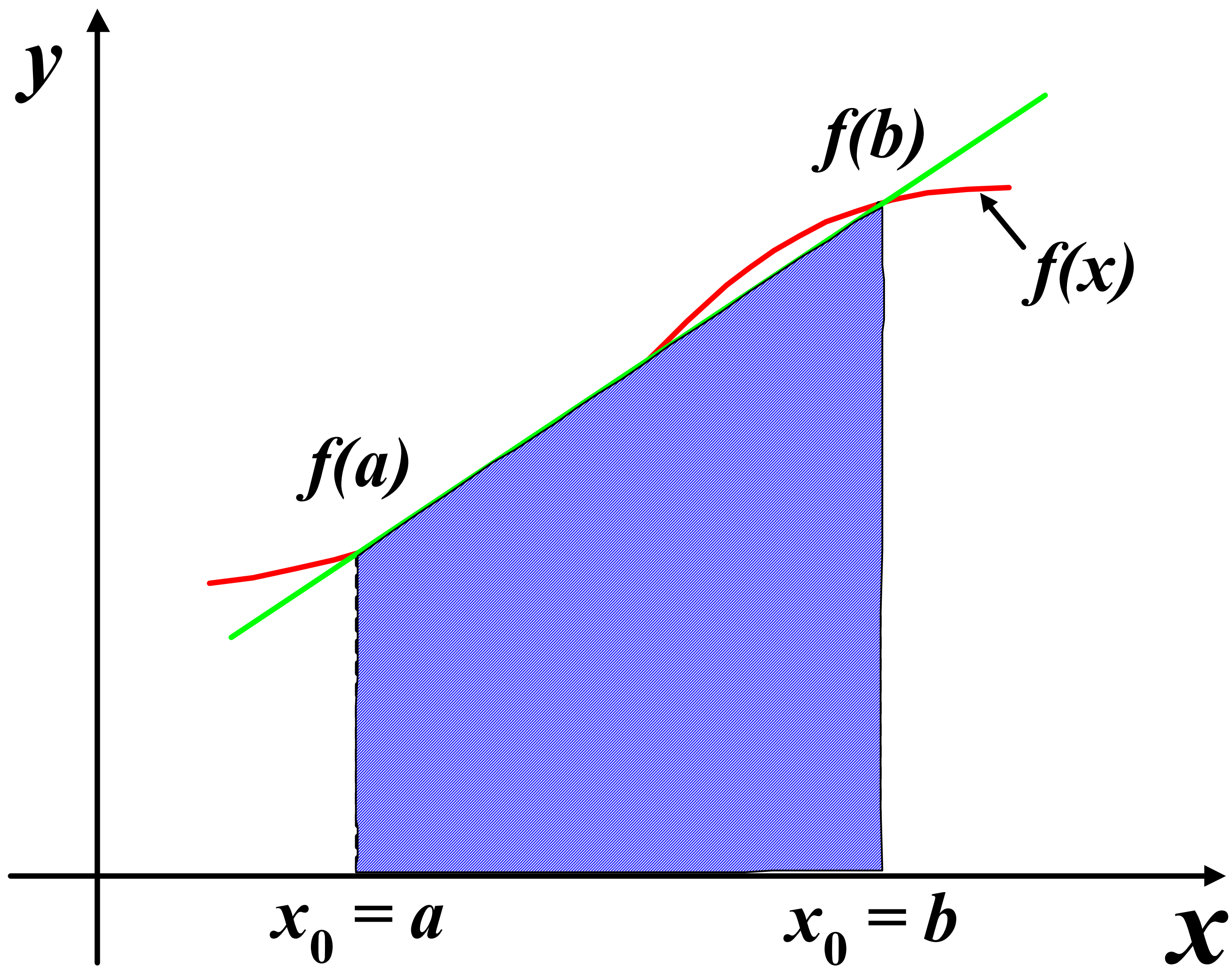
$$= 3.2$$

NUMERICAL INTEGRATION

$\int_a^b f(x)dx =$ area under the curve *f(x)* between $x = a$ to $x = b$.

In many cases a mathematical expression for *f(x)* is unknown and in some cases even if *f(x)* is known its complex form makes it difficult to perform the integration.


y
f(b)
f(a)
f(x)
$x_0 = a$
$x_0 = b$
x


y
f(b)
f(x)
f(a)
$x_0 = a$
$x_0 = b$
x

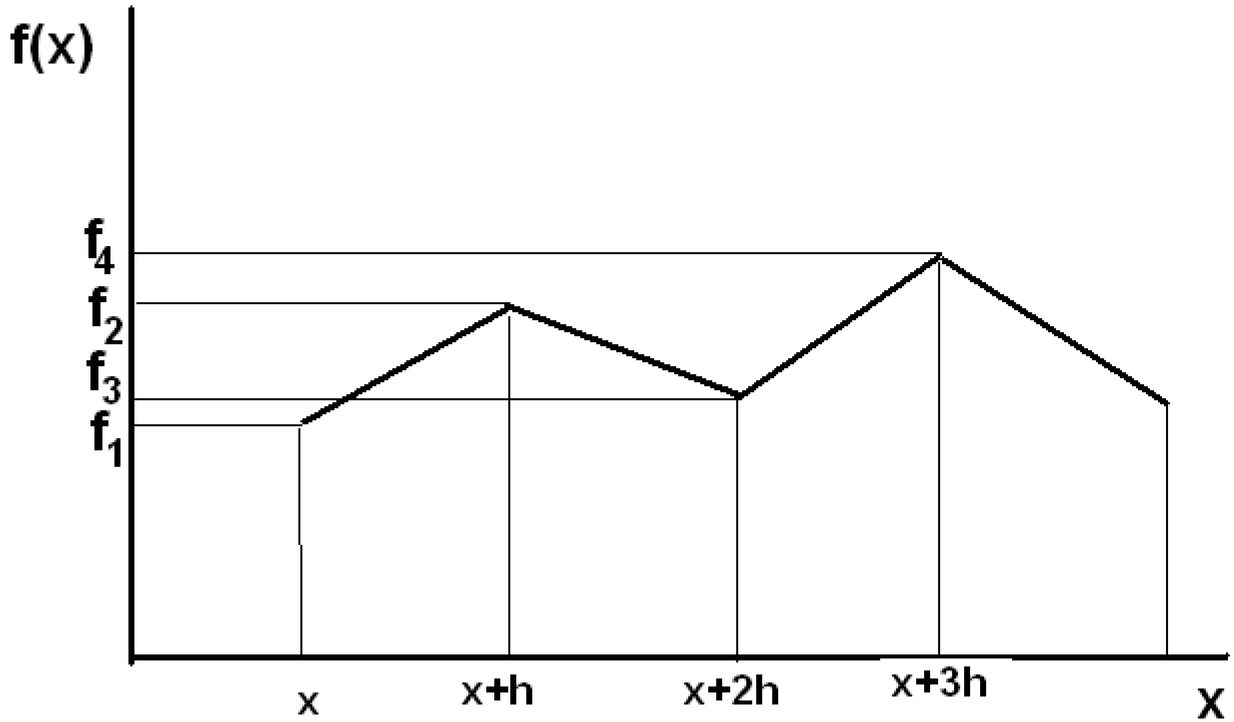
Area of the trapezoid

The length of the two parallel sides of the trapezoid are: ***f(a)*** **and** ***f(b)***

The height is ***b-a***

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

$$= \frac{h}{2}\left[f(a)+f(b)\right]$$



$$\int_{x_1}^{x_n} f(x)dx = \sum_{i=1}^{n} \frac{(f_i + f_{i+1})}{2} h = h(\frac{f_1}{2} + f_2 + f_3 + \ldots\ldots + \frac{f_{n+1}}{2})$$

Trapezoidal rule for integration

x	Angle(radian)	Sinx
x1	0.25	0.2474
x2	0.26	0.2571
x3	0.27	0.2667
x4	0.28	0.2764
x5	0.29	0.2860

$$\int_{0.25}^{0.29} \sin x dx = \left(\frac{0.2474}{2} + 0.2571 + 0.2667 + 0.2764 + \frac{0.2860}{2} \right) \times 0.01$$

$$= 0.010669$$

Using Trapezoidal rule solve the integral,

$$\int_0^1 \frac{1}{x^2+6x+10}\,dx$$

with four subintervals.

Using Trapezoidal rule solve the integral,

$$\int_0^1 \frac{1}{x^2+6x+10}\,dx$$

with four subintervals.

$$\int_0^1 \frac{1}{x^2+6x+10}\,dx = \frac{0.25}{2}\left[0.10 + 2\times 0.08649 + 2\times 0.07547 + 2\times 0.06639 + 0.05882\right]$$

$$= 0.07694.$$

Simpson's 1/3 Rule (quadratic interpolating polynomial)

$$\int_{x_0}^{x_2} f(x)\,dx \approx \int_{x_0}^{x_2} P(x)\,dx$$

$$\boldsymbol{x}_1 = \boldsymbol{x}_0 + \boldsymbol{h} \ \textbf{ and } \ \boldsymbol{x}_2 = \boldsymbol{x}_0 + 2\boldsymbol{h}$$

$$\int_{x_0}^{x_2} P(x)\,dx = \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0)\,dx$$

$$+\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1)\,dx$$

$$+\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)\,dx$$

$$\int_{x_0}^{x_2} f(x)dx \approx \int_{x_0}^{x_2} P(x)dx$$

$$= \frac{h}{3}\left[f\left(x_0\right) + 4f(x_1) + f(x_2)\right]$$

$$\int_{x_0}^{x_n} P(x)dx = \frac{h}{3}\left[f_1 + 4f_2 + 2f_3 + 4f_4 + \ldots\ldots\ldots\ldots\ldots + f_{n+1}\right]$$

$$f(x) = 5x^3 - 3x^2 + 2x + 1$$

Integrate the above function from x=-1 to x=1 using Simpson's rule with h=1

$$\int_{-1}^{1} P(x)dx = \frac{1}{3}\left[f_{-1} + 4f_0 + f_1\right] = 0$$

Compute the integral $I = \sqrt{\frac{2}{\pi}} \int_0^1 e^{-x^2/2} dx$ using Simpson's 1/3 rule, taking h = 0.125.

Compute the integral $I = \sqrt{\frac{2}{\pi}} \int_0^1 e^{-x^2/2} dx$ using Simpson's 1/3 rule, taking h = 0.125.

j	x_j	$f_j = f(x_j) = \sqrt{\frac{2}{\pi}} e^{-x_j^2/2}$		
0	0.000	0.7979		
1	0.125		0.7917	
2	0.250			0.7733
3	0.375		0.7437	
4	0.500			0.7041
5	0.625		0.6563	
6	0.750			0.6023
7	0.875		0.5441	
8	1.000	0.4839		
Sums		s_0=1.2818	s_1=2.7358	s_2=2.0797

j	x_j	$f_j = f(x_j) = \sqrt{\frac{2}{\pi}} e^{-x_j^2/2}$		
0	0.000	0.7979		
1	0.125		0.7917	
2	0.250			0.7733
3	0.375		0.7437	
4	0.500			0.7041
5	0.625		0.6563	
6	0.750			0.6023
7	0.875		0.5441	
8	1.000	0.4839		
Sums		s_0=1.2818	s_1=2.7358	s_2=2.0797

$$I = \sqrt{\frac{2}{\pi}} \int_0^1 e^{-x^2/2} dx = \frac{0.125}{3}\left[1.2818 + 4(2.7358) + 2(2.0797)\right]$$

$$= 0.6827$$

Simpson's 3/8 Rule (cubic interpolating polynomial)

$$\int_{x_0}^{x_3} f(x)\,dx \approx \frac{3}{8}h\left(f_0 + 3f_1 + 3f_2 + f_3\right)$$

$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h$$

$$x_3 = x_0 + 3h$$