NUMERICAL INTERGRATION

NUMERICAL INTEGRATION

INTRODUCION TO QUADRATURE

We approach the subject of numerical integration. The goal is to approximate the definite integral of f(x) over the interval [a,b] by evaluating f(x) at a finite number of sample points.

DEFINITION: Suppose that $a = x_0 < x_1 <\ldots< x_M = b$. A formula of the form

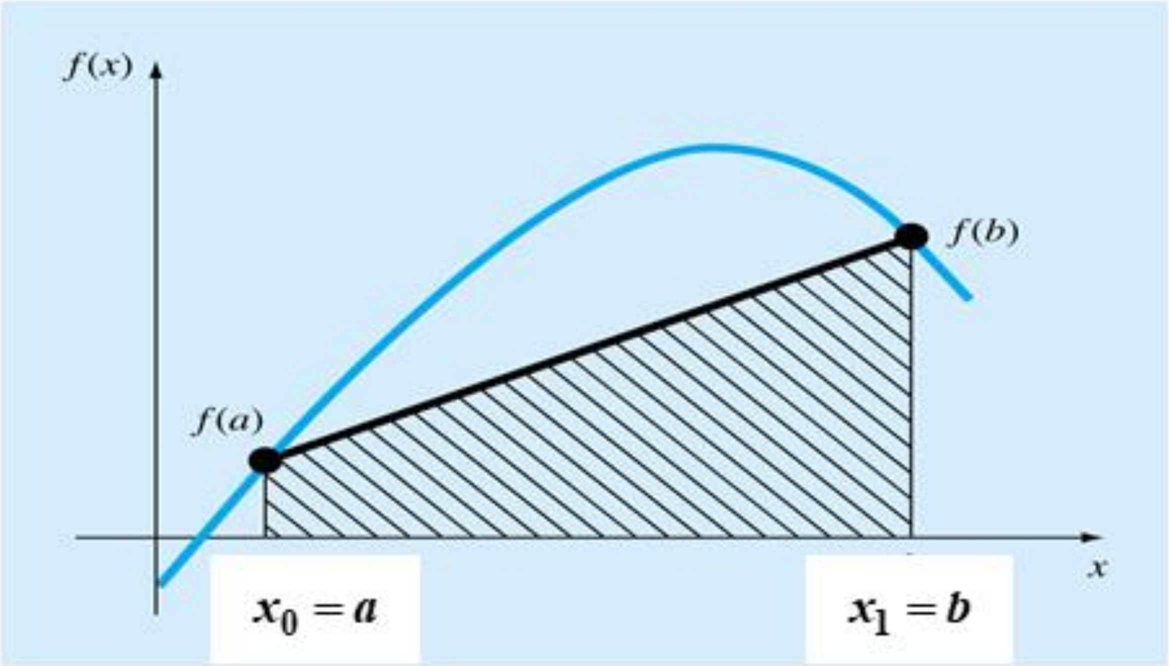
$$Q[f] = \sum_{k=0}^{M} w_k f(x_k) = w_0 f(x_0) + w_1 f(x_1) +\ldots+ w_M f(x_M \Big)$$

$$with\ \ property\ \ that$$

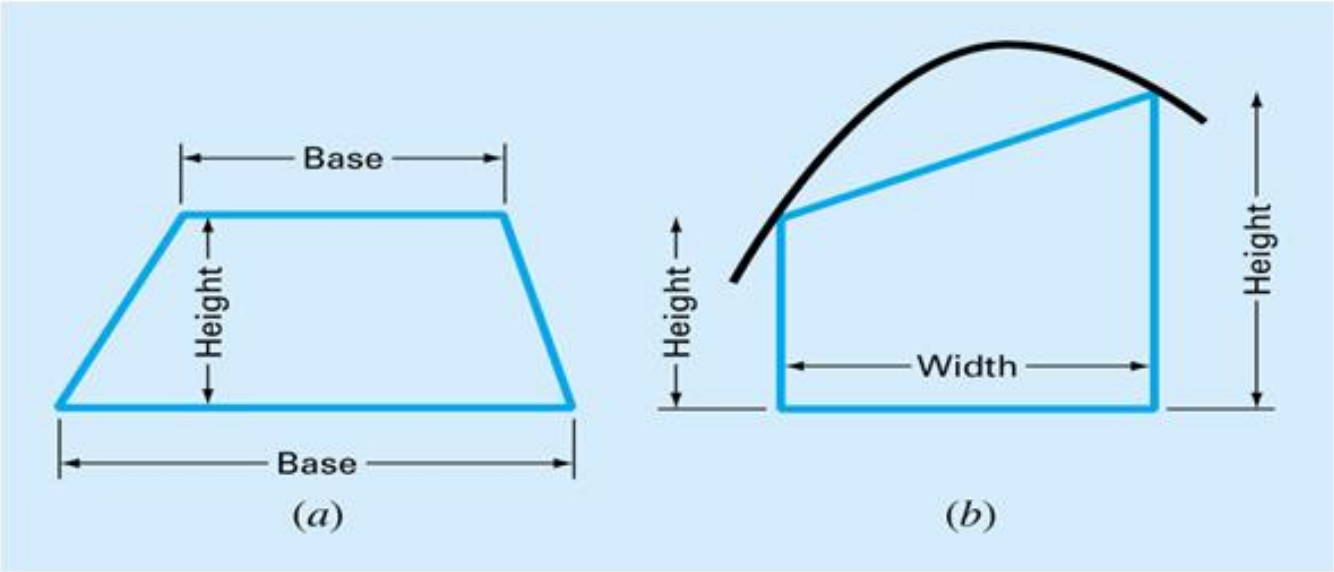
$$\int_a^b f(x)dx = Q[f] + E[f]$$

is called a numerical integration or quadrature formula. The term E[f] is called the truncation error for integration. The values $\{x_k\}_{k=0}^{M}$ are called the quadrature nodes , and $\{w_k\}_{k=0}^{M}$ are called the weights.

TRAPEZOIDAL RULE



Geometrically, the trapezoidal rule is equivalent to approximating the area of the trapezoid under the straight line connecting f(a) and f(b).



a) The formula for computing the area of a trapezoid: height times the average of the bases.
b) For the trapezoidal rule, the concept is the same but the trapezoid is on its side.

- The trapezoidal rule is the first of the Newton-Cote rules closed integration formulas.
- It is applicable where the polynomial is first-order.
- The area under a straight line is an estimate of the integral of f(x) between the limits a and b.

- The result of this integration is called the trapezoidal rule

$$where \quad x_0 = a \quad and \quad x_1 = b \qquad and \quad h = b - a \quad , then$$

$$\int_{x_0}^{x_1} f(x)\ dx \approx \frac{h}{2}(f_0 + f_1) \qquad Trapezoidal \quad rule$$

Corollary: Assume that f(x) is sufficiently differentiable; then $E[f]$ for Newton-Cotes quadrature involves an appropriate higher derivative. The trapezoidal rule has degree of precision n=1.
If $f \in C^2[a,b]$, then

$$\boxed{\int_{x_0}^{x_1} f(x)\ dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12} f^{(2)}(c\Big)}$$

PROOF

Proof for $\displaystyle\int_{x_0}^{x_1} f(x) \approx \frac{h}{2}(f_0 + f_1)$

Use first order Lagrange Interpolation

$$f(x) = f_0 \frac{(x - x_1)}{(x_0 - x_1)} + f_1 \frac{(x - x_0)}{(x_1 - x_0)}$$

$$\int_{x_0}^{x_1} f(x)\ \ dx = f_0 \int_{x_0}^{x_1} \frac{(x - x_1)}{(x_0 - x_1)} dx + f_1 \int_{x_0}^{x_1} \frac{(x - x_0)}{(x_1 - x_0)} dx$$

$$Let\;\; x = x_0 + th \quad \Rightarrow \quad dx = h\,dt \quad where \quad 0 \le t \le 1$$

$$x_0 = x_0 + 0h$$

$$x_1 = x_0 + h$$

$$\int_{x_0}^{x_1} f(x)\; dx = f_0 \int_0^1 \frac{h(t-1)}{-h} h\; dt + f_1 \int_0^1 \frac{th}{h} h\; dt = \ldots = \frac{h}{2}[f_0 + f_1] \quad (exercise)$$

ERROR ESTIMATE FOR THE TRAPEZOIDAL RULE

THEOREM: Let $f \in C^2[x_0, x_1]$. The error that the trapezoidal rule makes in estimating

$\int_{x_0}^{x_1} f(x)\; dx$ **is** $\boxed{E_{Trap} = \frac{-h^3}{12} f^{(2)}(c)}$ $where \;\; h = x_1 - x_0$

Proof:

From the Lagrange interpolation formula with remainder

$$f(x) = P_n(x) + \frac{f^{(n+1)}(c)}{(n+1)!)} \prod_{j=0}^{n} (x - x_j) \quad \text{then}$$

$$\int_{x_0}^{x_1} f(x)\ dx = \frac{h}{2}[f_0 + f_1] + \frac{f^{(n+1)}(c)}{(n+1)!)} \int_{x_0}^{x_1} \prod_{j=0}^{n} (x - x_j)\, dx$$

where n=1

$$\int_{x_0}^{x_1} f(x)\ dx = \frac{h}{2}[f_0 + f_1] + \frac{f^{(2)}(c)}{2!} \int_{x_0}^{x_1} (x - x_0)(x - x_1) dx$$

$$Let\ \ x = x_0 + th \quad \Rightarrow \quad dx = h\,dt \quad where \quad 0 \le t \le 1$$

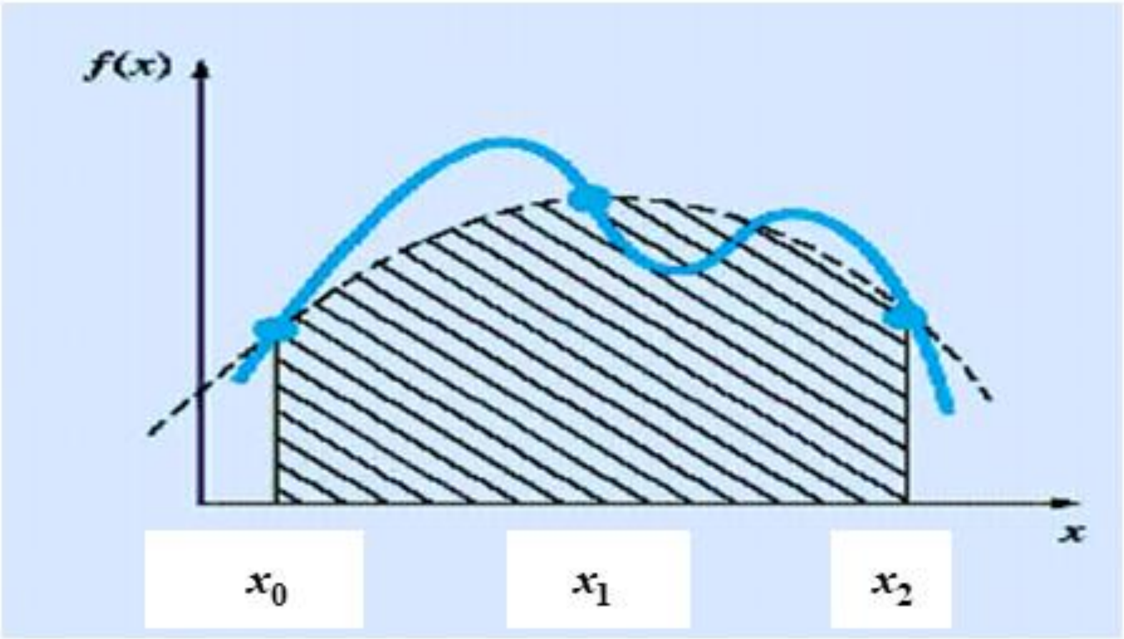
$$x_0 = x_0 + 0h$$

$$x_1 = x_0 + h$$

$$E_{Trap}(f) = \frac{f^{(2)}(c)}{2!}\int_{x_0}^{x_1}(x - x_0)(x - x_1)dx = \frac{f^{(2)}(c)}{2!}\int_0^1 th(t-1)h\ hdt = -\frac{h^3 f^{(2)}(c)}{12}$$

$\frac{1}{3}$ AND $\frac{3}{8}$ SIMPSON'S RULE

1. Simpson's 1/3 rule : It consists of taking the area under a parabola connecting three points.



where
$$\boxed{\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left(f_0 + 4f_1 + f_2\right) - \frac{h^5}{90} f^{(4)}(c)}$$

Proof for

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left(f_0 + 4f_1 + f_2\right)$$

Use Lagrange Interpolation polynomial

$$\int_{x_0}^{x_2} f(x)\,dx = f_0\int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}dx + f_1\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}dx + f_2\int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}dx$$

$$Let\quad x = x_0 + th \quad \Rightarrow \quad dx = h\,dt \quad where \quad 0 \le t \le 2$$

$$x_0 = x_0 + 0h$$

$$x_1 = x_0 + h$$

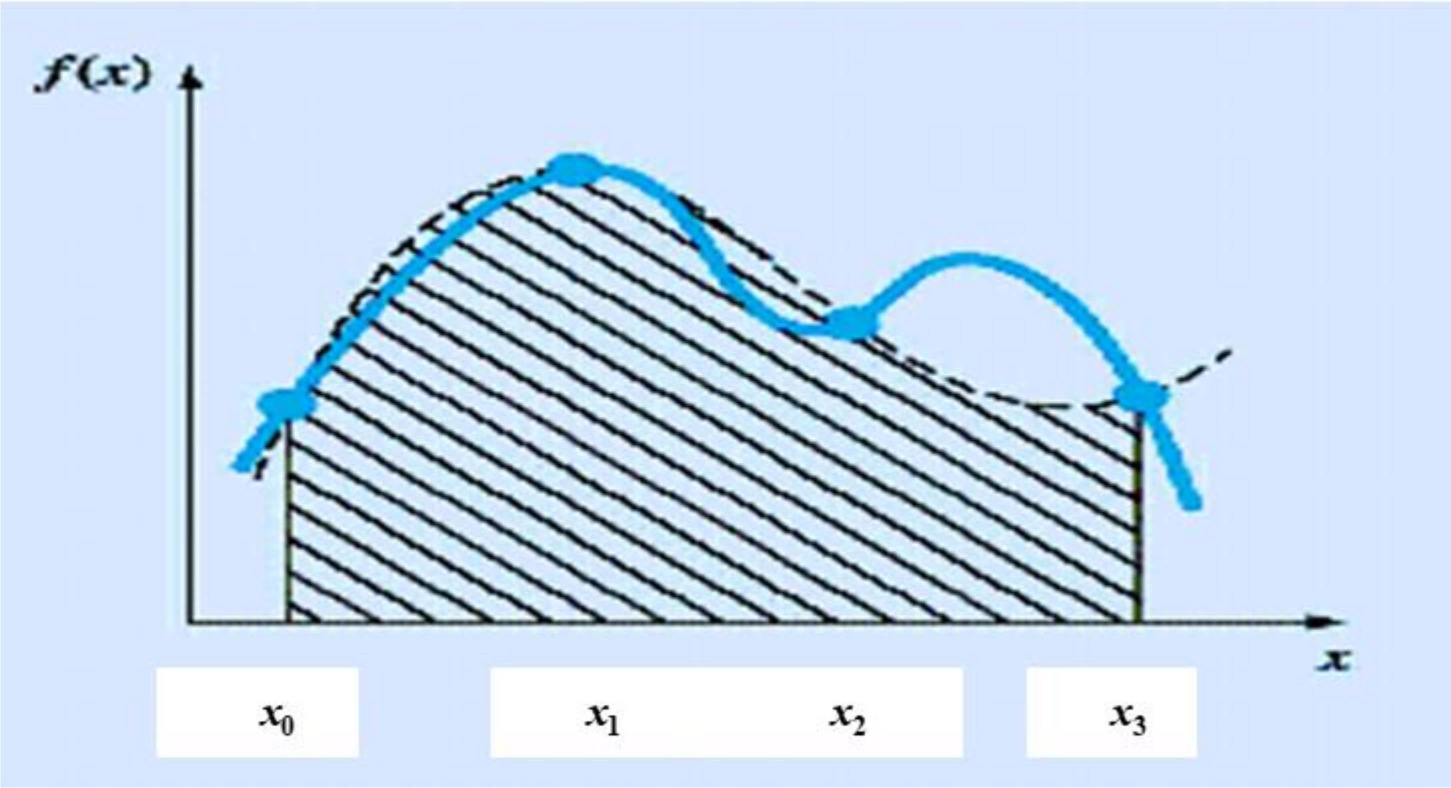
$$x_2 = x_0 + 2h$$

then

$$\int_0^2 f(x)dx = f_0\int_0^2 \frac{h(t-1)h(t-2)h\,dt}{(-h)(-2h)} + f_1\int_0^2 \frac{th\;h(t-2)h\,dt}{(h)(-h)} + f_2\int_0^2 \frac{th\;h(t-1)h\,dt}{(2h)(h)} \qquad \textbf{(exercise)}$$

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left(f_0 + 4f_1 + f_2\right)$$

2. Simpson's 3/8 rule: It consists of taking the area under a cubic equation connecting four points.



where $$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}\left(f_0 + 3f_1 + 3f_2 + f_4\right) - \frac{3h^5}{80} f^{(4)}(c)$$

Example: Evaluate the integral of the following data

x	0	0.1	0.2	0.3
f(x)	1	7	4	3

with the

a) Trapezoidal rule
b) Trapezoidal and $1/3$ Simpson's rule
c) $3/8$ Simpson's rule

where h=0.1

a)

$$\int_0^{0.3} f(x)\,dx = \frac{0.1}{2}(f_0+f_1)+\frac{0.1}{2}(f_1+f_2)+\frac{0.1}{2}(f_2+f_3)$$

$$=\frac{0.1}{2}(1+7)+\frac{0.1}{2}(7+4)+\frac{0.1}{2}(4+3)=1.3$$

b)

$$\int_{0}^{0.1} f(x)\,dx + \int_{0.1}^{0.3} f(x)\,dx + = \frac{0.1}{2}(f_0 + f_1) + \frac{0.1}{3}(f_1 + 4f_2 + f_3)$$

$$= \frac{0.1}{2}(1+7) + \frac{0.1}{3}(7 + 4(4) + 3) = 1.26666$$

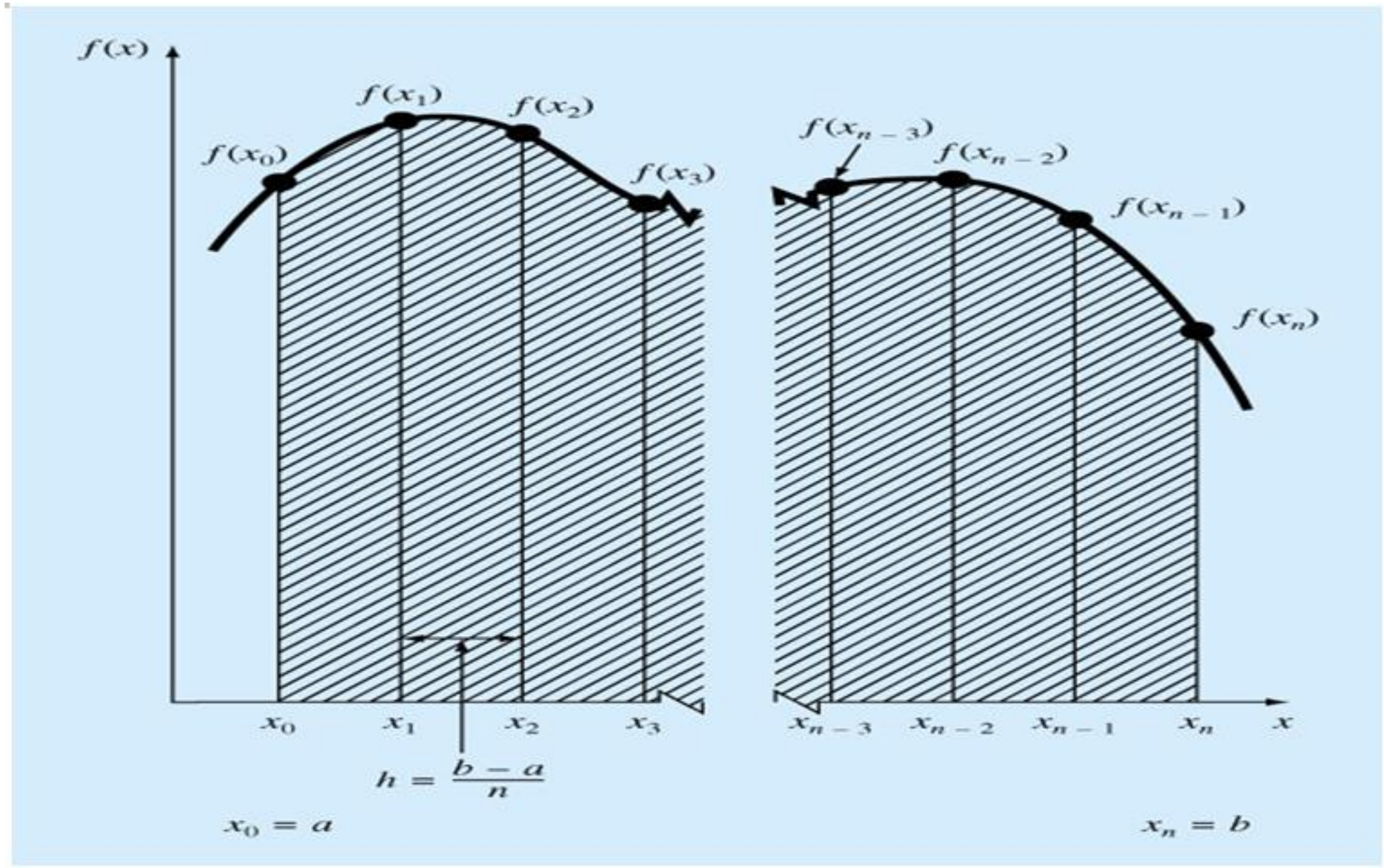
c)

$$\int_{0}^{0.3} f(x)\,dx = \frac{3(h)}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

$$= \frac{3(0.1)}{8}(1 + 3(7) + 3(4) + 3) = 1.3875$$

COMPOSITE TRAPEZOIDAL RULE

To improve the accuracy of the trapezoidal rule dividing the integration interval from a to b into a number of segments and apply the method to each segment.



Theorem: (Composite Trapezoidal Rule)

Suppose that the interval [a,b] is subdivided into M subinterval $\left[x_k, x_{k+1}\right]$ of width $h=\dfrac{(b-a)}{M}$ by using the equality spaced nodes $x_k = a + kh$, $\quad for \quad k = 0, 1, \ldots, M$. The composite trapezoidal rule for M subintervals can be expressed in any of three equivalent ways

$$T(f,h)=\frac{h}{2}\sum_{k=1}^{M}\left(f(x_{k-1})+f(x_k)\right) \quad \ldots\ldots\ldots\ldots\ldots\ldots(1)$$

$$T(f,h)=\frac{h}{2}(f_0+2f_1+2f_2+2f_3+\ldots+2f_{M-2}+2f_{M-1}+f_M) \quad \ldots\ldots\ldots(2)$$

$$T(f,h)=\frac{h}{2}(f(a)+f(b))+h\sum_{k=1}^{M-1}f(x_k) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

This is an approximation to the integral of $f(x)$ $over$ $[a,b]$, and we write

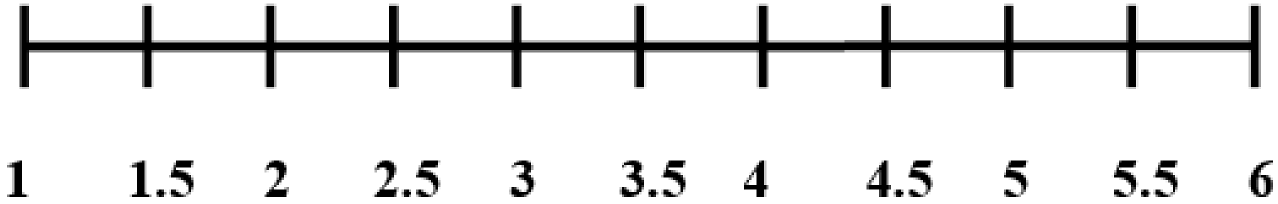
$$\int_a^b f(x)\,dx \approx T(f,h)$$

Example:

Consider $f(x) = 2 + \sin(2\sqrt{x})$. Use the composite trapezoidal rule with 11 sample points to compute an approximation to integral of $f(x)$ $\ taken\ \ over\ \ [1,6]$.

Solution

To generate 11 sample points we use M=10 that is $h = \frac{(6-1)}{10} = 0.5$



$$T(f,h) = \frac{h}{2}(f(a) + f(b)) + h\sum_{k=1}^{M-1} f(x_k)$$

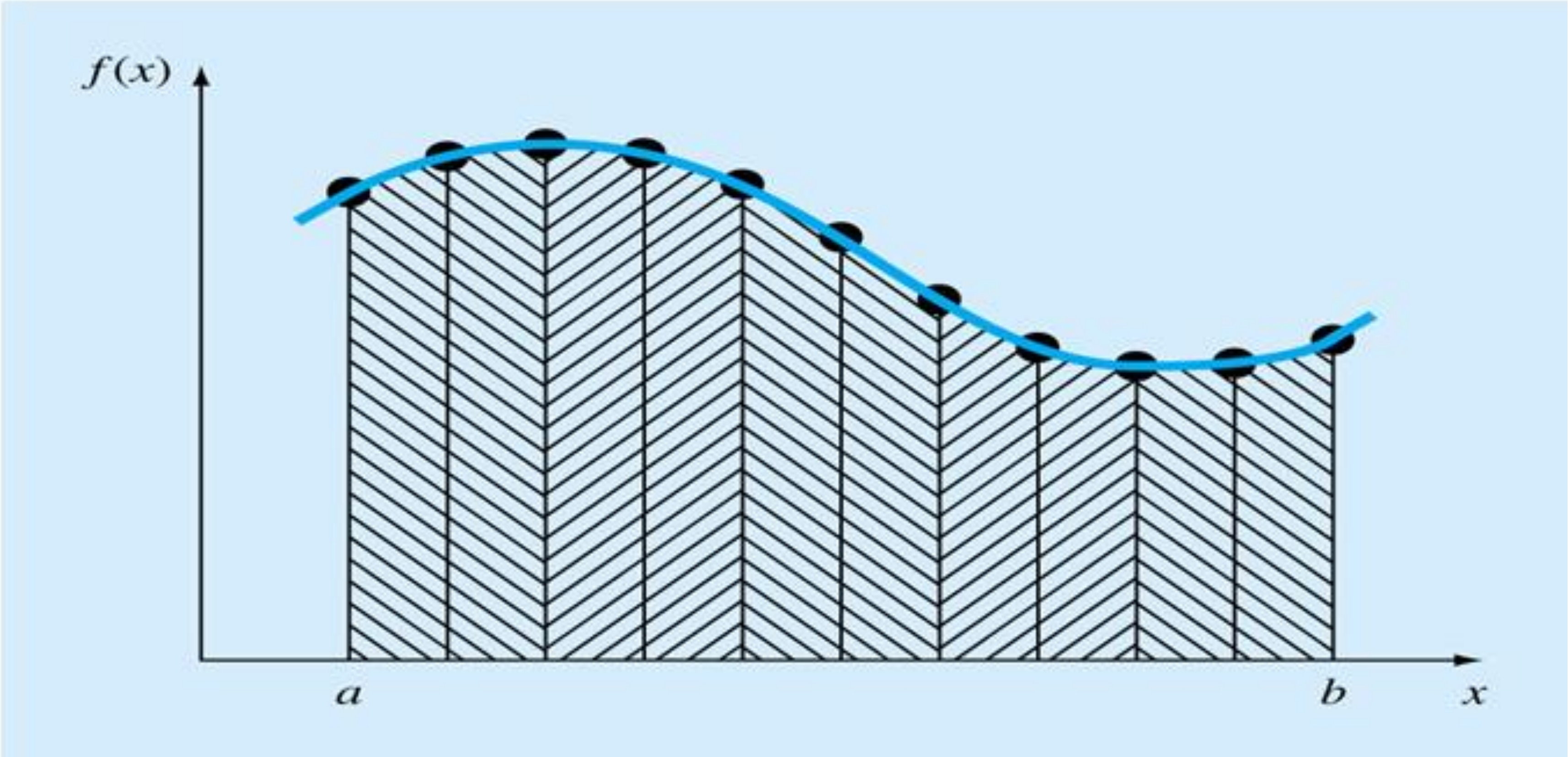
$$= \frac{0.5}{2}(f(1) + f(6)) + 0.5\big(f(1.5) + f(2) + f(2.5) + f(3) + f(3.5) + f(4) + f(4.5) + f(5) + f(5.5)\big)$$

$$= 8.19385457$$

COMPOSITE SIMPSON RULE

- Simpson's 1/3 rule can be improved by dividing the integration interval into a number of segments of equal width

- This method can be employed only if the number of segments is <u>even</u>.



THEOREM: (Composite Simpson Rule)

Suppose that the interval [a,b] is subdivided into 2M subinterval $[x_k, x_{k+1}]$ of width $h = \frac{(b-a)}{2M}$ by using the equality spaced nodes $x_k = a + kh$, $for \;\; k = 0,1,\ldots,2M$. The composite Simpson rule for 2M subintervals can be expressed in any of three equivalent ways

$$S(f,h) = \frac{h}{3}\sum_{k=1}^{M}\left(f(x_{2k-2}) + 4f(x_{2k-1}) + f(x_{2k})\right) \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

$$S(f,h) = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + \ldots + 2f_{2M-2} + 4f_{2M-1} + f_{2M}) \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

$$S(f,h) = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3}\sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3}\sum_{k=1}^{M} f(x_{2k-1}) \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots (3)$$

This is an approximation to the integral of $f(x)$ $over$ $[a,b]$, and we write

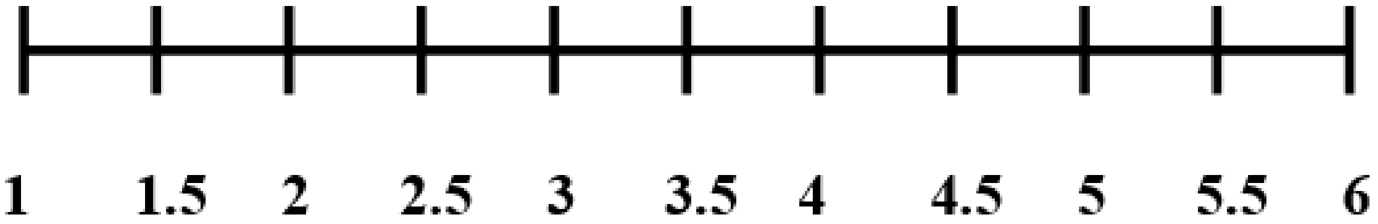
$$\int_a^b f(x)\,dx \approx S(f,h)$$

Example:

Consider $f(x) = 2 + \sin(2\sqrt{x})$. Use the composite Simpson rule with 11 sample points to compute an approximation to integral of $f(x)$ $taken\ \ over$ $[1,6]$.

Solution:

To generate 11 sample points we use M=5 that is $h = \frac{(6-1)}{2(5)} = 0.5$



$$S(f,h) = \frac{0.5}{3}[f(1) + f(6)] + \frac{2(0.5)}{3}\sum_{k=1}^{4} f(x_{2k}) + \frac{4(0.5)}{3}\sum_{k=1}^{5} f(x_{2k-1})$$

$$= \frac{1}{6}[f(1) + f(6)] + \frac{1}{3}[f(2) + f(3) + f(4) + f(5)] + \frac{2}{3}[f(1.5) + f(2.5) + f(3.5) + f(4.5) + f(5.5)]$$

$$= 8.1830155$$

ERROR ANALYSIS

COROLLARY : (Trapezoidal Rule Error Analysis)

Suppose that the interval [a,b] is subdivided into M subinterval $[x_k, x_{k+1}]$ of width $h = \frac{(b-a)}{M}$ by using the equality spaced nodes $x_k = a + kh\ ,\quad for\ \ k = 0,1,\ldots,M$. The composite trapezoidal rule

$$T(f,h) = \frac{h}{2}(f(a) + f(b)) + h\sum_{k=1}^{M-1} f(x_k)$$

is an approximation to the integral

$$\int_a^b f(x)\ dx \approx T(f,h) + E_T(f,h)$$

Furthermore, if $f \in C^2[a,b]$, there exists a value $c \quad with \quad a < c < b$ so that the error term $E_T(f,h)$ has the form

$$E_T(f,h) = \frac{-(b-a)f^{(2)}(c)h^2}{12} = O(h^2)$$

Example: Find the number M and step size h so that the error $E_T(f,h)$ for the composite trapezoidal rule is less than 5×10^{-9} for the approximation

$$\int_2^7 \frac{dx}{x} \approx T(f,h\Big)$$

Solution:

Where, $f(x)=\frac{1}{x}$, $f'(x)=\frac{-1}{x^2}$ and $f''(x)=\frac{2}{x^3}$

The maximum value of $f''(x)=\frac{2}{x^3}$ $over$ [2,7] occur at x=2, that is

$$|f''(2)|=\frac{1}{4} \quad for \quad 2<c<7. \qquad |E_T(f,h)|\le\left|\frac{-(b-a)f^{(2)}(c)h^2}{12}\right|\le 5\times10^{-9}$$

$$\left|\frac{-(7-2)\frac{1}{4}h^2}{12}\right|\le 5\times10^{-9} \quad\Rightarrow\frac{5h^2}{48}\le 5\times10^{-9}\Rightarrow h^2\le\frac{48(5\times10^{-9})}{5}$$

$$h\approx 2.19089\times10^{-4} \quad then \quad h=\frac{(b-a)}{M} \quad\Rightarrow M=\frac{5}{2.19089\times10^{-4}}=22821.77323$$

M must be integer $\boxed{M\approx 22822}$

COROLLARY: (Simpson's Rule Error Analysis)

Suppose that the interval [a,b] is subdivided into 2M subinterval $[x_k, x_{k+1}]$ of width $h = \frac{(b-a)}{2M}$ by using the equality spaced nodes $x_k = a + kh$, $for \; k = 0,1, \ldots, 2M$. The composite Simpson rule

$$S(f,h) = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3}\sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3}\sum_{k=1}^{M} f(x_{2k-1})$$

is an approximation to the integral

$$\int_a^b f(x)\, dx \approx S(f,h) + E_S(f,h))$$

Furthermore, if $f \in C^4[a,b]$, there exists a value $c \quad with \quad a < c < b$ so that the error term $E_S(f,h)$ has the form

$$E_S(f,h) = \frac{-(b-a)f^{(4)}(c)h^4}{180} = O(h^4))$$

Example : Find the number M and step size h so that the error $E_S(f,h)$ for the composite Simpson rule is less than 5×10^{-9} for the approximation

$$\int_{\frac{-\pi}{6}}^{\frac{\pi}{6}} \cos x \; dx \approx S(f,h\Big)$$

Solution:

$$|E_S(f,h)| \le \frac{|(b-a)|\left|f^{(4)}(c)\right|h^4}{180} \le 5 \times 10^{-9} \qquad where, f(x) = \cos x \quad then \quad f^{(4)}(x) = \cos x$$

Maximum value of $f^{(4)}(x) = \cos x$ occur when $x = 0 \;\; over \;\; \left[\frac{-\pi}{6}, \frac{\pi}{6}\right]$ that is $|\cos 0| = 1$

$$\frac{\left|\left(\frac{\pi}{6} - \frac{-\pi}{6}\right)\right| |1| h^4}{180} \le 5 \times 10^{-9} \quad \Rightarrow h^4 \le \frac{5 \times 10^{-9}(180)(3)}{\pi} \quad \Rightarrow h \approx 0.030447$$

$$where, \qquad h = \frac{b-a}{2M} \quad \Rightarrow \quad M = \frac{\frac{\pi}{6} - \left(\frac{-\pi}{6}\right)}{2(0.030447)} = \frac{\pi}{6(0.030447)} = 17.2$$

$\boxed{M \approx 18}$ Number of subintervals should be divisible by 2.

Example (exam question)

Evaluate $\int_{2.1}^{3.1} \frac{1}{x^2}\, dx$ using Composite Trapezoidal Rule with an error bound by 2×10^{-3} .

Solution:

First find h and M $\quad |E_T(f,h)| \leq \left|\frac{-(b-a)f^{(2)}(c)h^2}{12}\right| \leq 2 \times 10^{-3}$

$where\ \ f(x) = \frac{1}{x^2} \quad and \quad f^{(2)}(x) = \frac{6}{x^4}$ maximum occur at x=2.1 $\left|f^{(2)}(2.1)\right| = \left|\frac{6}{(2.1)^4}\right| = 0.3085$ then

$$\left|\frac{-(3.1-2.1)0.3085\, h^2}{12}\right| \leq 2 \times 10^{-3} \Rightarrow h^2 \leq 0.07779$$

2.1 2.35 2.6 2.85 3.1

$$h \approx 0.2789 \quad \Rightarrow M = \frac{3.1-2.1}{0.2789} = 3.58 \quad take \quad M = 4 \quad and \quad h = 0.25$$

$$T(f,h) = \frac{0.25}{2}[f(2.1) + f(3.1)] + 0.25[f(2.35) + f(2.6) + f(2.85)] = 0.15437675$$

Exact Value: $\int_{2.1}^{3.1} \frac{1}{x^2}\, dx = 0.1536$

Example: Apply Simpson's $\frac{1}{3}$ and Trapezoidal for $\int_0^1 e^{1-x^2}\,dx$. Using $h = 0.25$ and comment on the error bound and also on the error by Trapezoidal and Simpson's $\frac{1}{3}$ formula.

Solution:

For Trapezoidal:

$f(x) = e^{1-x^2}$, $h = 0.25$ on $[0,1]$

0	0.25	0.5	0.75	1

$$\int_{0}^{1} f(x)\,dx = \int_{0}^{0.25} f(x)\,dx + \int_{0.25}^{0.5} f(x)\,dx + \int_{0.5}^{0.75} f(x)\,dx + \int_{0.75}^{1} f(x)\,dx$$

$$= \frac{h}{2}[f_0 + f_1] + \frac{h}{2}[f_1 + f_2] + \frac{h}{2}[f_2 + f_3] + \frac{h}{2}[f_3 + f_4]$$

$$= \frac{h}{2}[f_0 + 2f_1 + 2f_2 + 2f_3 + f_4]$$

$$= \frac{h}{2}\left[f(0) + 2f(0.25) + 2f(0.5) + 2f(0.75) + f(1)\right]$$

$$= \frac{1}{4}\frac{1}{2}[2.718282 + 5.107179 + 4.234 + 3.097661 + 1]$$

$$= 2.01964$$

The error for Trapezoidal formula,

$$f(x) = e^{1-x^2}, \; f'(x) = -2xe^{1-x^2}, \; f''(x) = \left(4x^2 - 2\right)e^{1-x^2}$$

$$f''(0) = \left(4(0)^2 - 2\right)e^{1-(0)^2} = -5.4366$$

$$f''(1) = \left(4(1)^2 - 2\right)e^{1-(1)^2} = 2$$

The error is $E_1(x) = -\frac{h^3}{12}f''(c) - \frac{h^3}{12}f''(c) - \frac{h^3}{12}f''(c) - \frac{h^3}{12}f''(c) = -\frac{4h^3}{12}f''(c)$

$$\left|E_1(x)\right| = \frac{4h^3}{12}\left|f''(c)\right| = \frac{4(0.25)^3}{12}\left|-5.4366\right| = 0.02831$$

For Simpson's $\frac{1}{3}$:

$f(x) = e^{1-x^2}$, $h = \frac{1}{2N} = 0.25 = \frac{1}{4} = \frac{1}{(2)(2)}$ on $[0,1]$. $N = 2$ is the number of times of apply Simpson's.

0 0.25 0.5 0.75 1

$$\int_0^1 f(x)\,dx = \int_0^{0.5} f(x)\,dx + \int_{0.5}^1 f(x)\,dx$$

$$= \frac{h}{3}[f_0 + 4f_1 + f_2] + \frac{h}{3}[f_2 + 4f_3 + f_4]$$

$$= \frac{h}{3}[f_0 + 4f_1 + 2f_2 + 4f_3 + f]$$

$$= \frac{1}{4}\frac{1}{3}[f(0) + 4f(0.25) + 2f(0.5) + 4f(0.75) + f(1)]$$

$$= \frac{1}{12}[2.718282 + 10.214358 + 4.234 + 6.195321 + 1]$$

$$= 2.030163$$

$$\int_0^1 f(x)\,dx = 2.030163$$

$$f(x)=e^{1-x^2}\ ,\ f'(x)=-2xe^{1-x^2}\ ,\ f''(x)=\left(4x^2-2\right)e^{1-x^2}\ ,$$

$$f'''(x)=8xe^{1-x^2}-2x\left(4x^2-2\right)e^{1-x^2}=\left(-8x^3+12x\right)e^{1-x^2}$$

$$f^{(4)}(x)=\left(-24x^2+12\right)e^{1-x^2}-2x\left(-8x^3+12x\right)e^{1-x^2}=\left(16x^4-48x^2+12\right)e^{1-x^2}$$

$$\left|f^{(4)}(0)\right|=\left|\left(16(0)^4-48(0)^2+12\right)e^{1-(0)^2}\right|=32.6194$$

$$\left|f^{(4)}(1)\right|=\left|\left(16(1)^4-48(1)^2+12(1)\right)e^{1-(1)^2}\right|=20$$

$$E_2(x)=-\frac{h^5}{90}f^{(4)}(c)-\frac{h^5}{90}f^{(4)}(c)=-\frac{2h^5}{90}f^{(4)}(c)$$

$$\left|E_2(x)\right|=\frac{2h^5}{90}\left|f^{(4)}(c)\right|=\frac{2(0.25)^5}{90}(32.6194)=0.0007078$$

EXERCISE (E.Q): Determine the number M and h so that the composite Simpson rule for 2M subinterval can be used to compute the given integral with an accuracy of 10^{-3}

$$\int_0^2 (e^x + 3x^4)dx$$

EXERCISE(E.Q): Approximate the area A defined by $2\pi \int_a^b \sqrt{1+\left(f'(x)\right)^2}\ dx$ taking $f(x) = x^3$ for $0 \le x \le 1$ by using the Composite Trapezoidal rule with 5 subintervals.

EXERCISE (E.Q): Compute $\int_0^1 (8x^3 - 3x)\ dx$ using the Composite Trapezoidal rule, your results should be accurate to $\varepsilon = 5 \times 10^{-1}$.

EXERCISE : Page 374-375 Question : 3, 8, 9