NUMERICAL INTEGRATION (Numerical evaluation of integrals)

Complicated Integrals: $\int_0^1 e^{-x^2} dx$ or $\int_0^{\pi} x^{\pi} \sin(\sqrt{x})\, dx$ etc

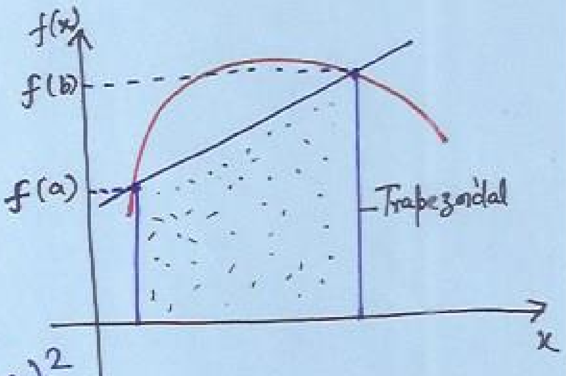
Newton's Cotes Integration formulas:

These formulas are based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate.

$$I = \int_a^b f(x)\,dx \simeq \int_a^b P_n(x)\,dx$$

where $P_n(x) = a_0 + a_1 x + \cdots + a_n x^n$

(1) The trapezoidal Rule: (Single application)



$$I = \int_a^b f(x)\,dx \simeq \int_a^b P_n(x)\,dx$$

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

$$= f(a)(b-a) + \frac{f(b)-f(a)}{b-a} \cdot \frac{1}{2}(b-a)^2$$

$$= f(a)(b-a) + \frac{1}{2}(b-a)\cdot(f(b)-f(a))$$

$$\Rightarrow \boxed{\int_a^b f(x)\,dx \simeq (b-a)\frac{[f(a)+f(b)]}{2}}$$

Problem: Using trapezoidal rule integral numerically the function $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $a=0$ to $b=0.8$. Compare result with exact value of integral 1.640533.

Solution: The function values

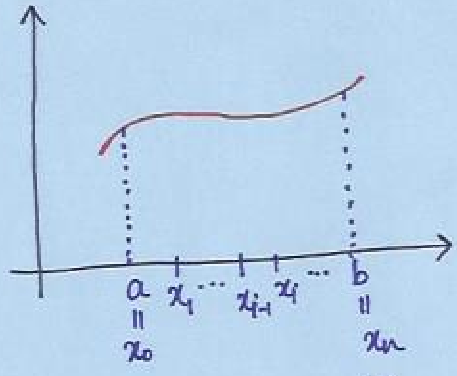
$$f(0) = 0.2$$

$$f(0.8) = 0.232$$

$$\int_0^{0.8} f(x)\,dx \simeq \frac{0.2 + 0.232}{2}(0.8 - 0) = 0.1728$$

The multiple-application of Trapezoidal Rule

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



Consider there are $n+1$ equally spaced base points $x_0, x_1, \ldots, x_n$.

Then, $$h = \frac{b-a}{n}$$

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

$$\simeq h\,\frac{f(x_0) + f(x_1)}{2} + h\,\frac{f(x_1) + f(x_2)}{2} + \ldots + h\,\frac{f(x_{n-1}) + f(x_n)}{2}$$

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

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

Problem: Use the two-segment trapezoidal rule to estimate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $a = 0$ to $b = 0.8$.

Solution:

$$0 \quad 0.4 \quad 0.8$$

$$h = \frac{0.8 - 0}{2} = 0.4$$

$f(0) = 0.2$, $f(0.4) = 2.456$, $f(0.8) = 0.232$

$$I = \int_0^{0.8} f(x)\,dx \simeq \frac{0.4}{2}\left[0.2 + 0.232 + 2(2.456)\right]$$

$$= 1.0688 \text{ Ans.}$$

Error Bounds for the trapezoidal Rule:

(1) Single application:

We know, $f(x) - P_1(x) = (x - x_0)(x - x_1)\dfrac{f''(t)}{2}$ ——(1)

with a suitable t depending on x between x_0 and x_1.

Integrating (1) from x_0 to $x_1 = x_0 + h$ gives.

$$E = \int_{x_0}^{x_0+h} f(x)\,dx - \frac{h}{2}\left[f(x_0) + f(x_1)\right] = \int_{x_0}^{x_0+h} (x - x_0)(x - x_1)\frac{f''(\overset{t(x)}{t})}{2}\,dx.$$

Applying weighted mean value theorem* ($(x-x_0)(x-x_1)$) does not change sign in $[x_0, x_0+h]$, we get

$$E = \frac{f''(\tilde{t})}{2}\int_{x_0}^{x_0+h} (x - x_0)(x_0 - x_0 - h)\,dx$$

Substitute $x - x_0 = v \Rightarrow dx = dv$

* last page 9

$$= \frac{f''(\tilde{t})}{2} \cdot \int_0^h v(v-h)\,dx = \frac{f''(\tilde{t})}{2} \cdot \left[\frac{1}{3}h^3 - \frac{h}{2} \cdot h^2\right]$$

$$= -\frac{h^3}{12} f''(\tilde{t}) \quad , \text{where } \tilde{t} \in (x_0, x_1)$$

Error in Multiple Application

$$E = \sum_{i=0}^{n-1} \left(-\frac{h^3}{12} f''(\tilde{t}_i)\right)$$

$$= -\frac{h^3}{12} \sum_{i=0}^{n-1} f''(\tilde{t}_i)$$

Using discrete mean value theorem: (see. last page 9)

$$= -\frac{h^3}{12} \cdot n \cdot f''(\hat{t})$$ with suitable, unknown $\hat{t}$ between a and b.

$$\boxed{E = -\frac{(b-a)}{12} h^2 f''(\hat{t})}$$

Error Bounds:

Let $M_2 = \max_{[x_0, x_n]} |f''(x)|$. Then,

$$\boxed{|E| \leq \frac{(b-a)h^2}{12} M_2}$$

Example: Evaluate the following integral using trapezoidal rule with $n = 2, 4$. Compare with the exact solution

$$\int_0^1 \frac{dx}{3+2x}.$$

Find the bound on the error. Also find the number of sub-intervals required if the error is to be less than 5×10^{-4}!

<u>Solution</u>: (i) Number of subintervals $=2$ i.e. $h=0.5=\dfrac{\overset{1}{\overset{\|}{b}}-\overset{0}{\overset{\|}{a}}}{\underset{\underset{2}{\|}}{n}}$

Hence, $$I_1 = \frac{0.5}{2}\left[f(0)+2f(0.5)+f(1)\right]$$

$$= \frac{0.5}{2}\left[\frac{1}{3}+2\cdot\frac{1}{4}+\frac{1}{5}\right]$$

$$= 0.25833$$

(ii) Number of subinterval $n=4$:

$$h=\frac{1-0}{4}=\frac{1}{4}$$

$x_0=0$, $x_1=\frac{1}{4}$, $x_2=\frac{2}{4}$, $x_3=\frac{3}{4}$, $x_4=1$.

Hence, $$I_2=\frac{1}{4}\cdot\frac{1}{2}\left[f(0)+2\left(f\left(\tfrac{1}{4}\right)+f\left(\tfrac{1}{2}\right)+f\left(\tfrac{3}{4}\right)\right)+f(1)\right)+f(1)\right]$$

$$=\frac{1}{8}\left[\frac{1}{3}+2\left(\frac{2}{7}+\frac{1}{4}+\frac{2}{9}\right)+\frac{1}{5}\right]$$

$$=0.25615$$

Exact Solution: $\frac{1}{2}\ln\left(\frac{5}{3}\right)=0.25541$

Errors: $$E_1=|0.25541-0.25833|$$

$$=0.00292$$

$$E_2=|0.25541-0.25615|=0.00074$$

<u>Errors Bounds</u>: $f(x)=\dfrac{1}{3+2x}$, $f'(x)=\dfrac{-2}{(3+2x)^2}$

$$f''(x)=\frac{8}{(3+2x)^3}$$

and $$M_2=\max_{[0,1]}\frac{8}{(3+2x)^3}=\frac{8}{27}$$

Hence, $|\text{Error}| \le \frac{(b-a)h^2}{12} M_2 = \frac{1}{\cancel{12}_3} h^2 \frac{\cancel{8}^2}{27}$

$$= \frac{2h^2}{81}$$

(i) for $h = 1/2$, $|\text{Error}| \le 0.00617$

(ii) for $h = 1/4$, $|\text{Error}| \le 0.00154$

Given, $E = 5 \times 10^{-4}$

$$\Rightarrow \frac{(b-a)h^2}{12} M_2 \le 5 \times 10^{-4}$$

$$\Rightarrow \frac{(b-a)(b-a)^2}{12 n^2} \cdot \frac{8}{27} \le 5 \times 10^{-4}$$

$$\Rightarrow \frac{1 \times 8}{12 \times 27 \times 5 \times 10^{-4}} \le n^2$$

$$\Rightarrow 49.38 \le n^2 \Rightarrow n \ge 7.03$$

Since, n is an integer, we require $n = 8$.

Simpson's 1/3 Rule

$$I = \int_a^b f(x)\,dx \approx \int_a^b P_2(x)\,dx.$$

let $x_0 = a$, x_1, $x_2 = b$

$$I \approx \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$

$$= \frac{1}{2h^2} f(x_0) \int_{x_0}^{x_2} (x-x_1)(x-x_1+x_1-x_2)\,dx$$

$$-\frac{1}{h^2} f(x_1) \int_{x_0}^{x_2} (x-x_0)(x-x_0+x_0-x_2)\,dx$$

$$+\frac{1}{2h^2} f(x_2) \int_{x_0}^{x_2} (x-x_0)(x-x_0+x_0-x_1)\,dx$$

$$= \frac{f(x_0)}{2h^2}\left[\frac{1}{3}(h^3+h^3)-h\cdot 0\right] - \frac{f(x_1)}{h^2}\left[\frac{1}{3}(2h)^3+\left(\frac{-2h}{3}\right)(2h)^2\right]$$

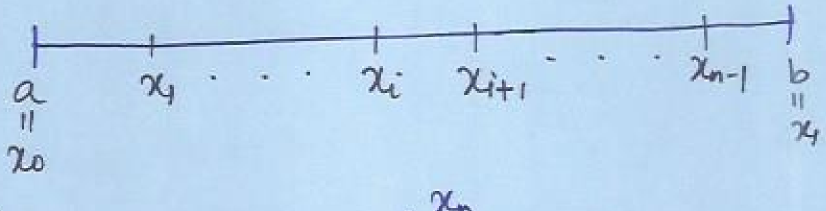
$$+\frac{f(x_2)}{2h^2}\left[\frac{1}{3}\cdot(2h)^3+\left(\frac{-h}{2}\right)(2h)^2\right]$$

$\vdots$

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

Multiple application of Simpson's Rule

$b-a=nh$



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

$$\simeq \frac{h}{3}\{f(x_0)+4f(x_1)+f(x_2)\} + \frac{h}{3}\{f(x_2)+4f(x_3)+f(x_4)\}$$

$$+\cdots+\frac{h}{3}\{f(x_{n-2})+4f(x_{n-1})+f(x_n)\}$$

$$= \frac{h}{3}\left[f(x_0)+4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)\right]$$

Error: Single application

$$E = -\frac{h^5}{90} f^{(4)}(\xi) \quad , \quad \xi \in (a,b)$$

or $\xi \in (x_0, x_2)$

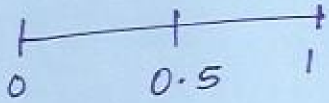
Multiple application

$$E = -\frac{b-a}{180} h^4 f^{(4)}(\xi) \quad , \quad \xi \in (a,b)$$

or $\xi \in (x_0, x_n)$

Example: Evaluate $\int_0^1 \frac{dx}{3+2x}$ using Simpson's rule with $n = 2, 4$. Compare with the Exact Solution.

Solution: $n=2$:



$$I \simeq \frac{h}{3}\left[f(0) + 4f\left(\tfrac{1}{2}\right) + f(1)\right]$$

$$= \frac{0.5}{3}\left[\frac{1}{3} + 4\cdot\frac{1}{4} + \frac{1}{5}\right]$$

$$= 0.25556$$

For $n=4$:

$$h = \frac{1}{4}$$

$$I \simeq \frac{h}{3}\left[f(0) + 4\left\{f\left(\tfrac{1}{4}\right) + f\left(\tfrac{3}{4}\right)\right\} + 2f\left(\tfrac{1}{2}\right) + f(1)\right]$$

$$= 0.25542 \text{ Ans}$$

Weighted mean value theorem:

Assume f and g are continuous in $[a,b]$.

If g never changes sign in $[a,b]$, then

$$\int_a^b f(x)\,g(x)\,dx = f(c)\int_a^b g(x)\,dx$$

where $c \in (a,b)$
& g is integrable.

Discrete mean value theorem:

Let $f \in C^0[a,b]$ and let x_j be $(n+1)$ points in $[a,b]$ and c_j be $(n+1)$ constants, all having the same sign. Then there exists $\xi \in [a,b]$ such that

$$\sum_{j=0}^{n} c_j f(x_j) = f(\xi)\sum_{j=0}^{n} c_j$$

In particular, if $c_j = 1 \;\forall j$

then

$$\boxed{\frac{1}{n+1}\sum_{j=0}^{n} f(x_j) = f(\xi)}$$