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# Numerical Integration



**Definite Integral:** The definite integral of a function over a fixed interval is a number. For example,

$$\int_0^2 x^2\,dx = \frac{8}{3}$$

or we can say that the value of definite integral of a function $f(x)$, which is a continuous function of $x$ in the interval $[a, b]$ is given by

$$\int_a^b f(x)\,dx = F(b) - F(a) \quad .$$

where $F(x)$ is the anti-derivative of $f(x)$ i.e., $F'(x) = f(x)$

The general problem of numerical integration may be stated as follows:

Given a set of data points $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$ of a function $y = f(x)$, where $f(x)$ is not known explicitly, it is required to compute the value of the definite integral

$$\int_a^b f(x)\,dx$$

Numerical quadrature is the process of computing the approximate value of a definite integral using a set of numerical values of the integrand where the interval of integration is finite.

Now, we derive the general quadrature formula as follows:

## Newton-Cote's Quadrature Formula:

Newton-Cote's quadrature formulas for approximating $\int_a^b f(x)dx$ are obtained by approximating the function of integration $f(x)$ by interpolating polynomials.

Let $I = \int_a^b f(x)\,dx$, where $f(x)$ takes the values $f_0, f_1, f_2, \ldots, f_n$ for $x = x_0, x_1, x_2, \ldots, x_n$. Let the interval of integration $[a,b]$ be divided into $n$ equal sub-intervals, each of width $h$, so that $x_0 = a,\ x_1 = x_0+h,\ x_2 = x_0+2h, \ldots, x_n = x_0+nh = b$

$$\therefore\ I = \int_{x_0}^{x_0+nh} f(x)\,dx$$

Since $x = x_0 + ph$ or $\frac{x-x_0}{h} = p \Rightarrow dx = h\,dp$

$$\therefore\ I = \int_{x_0}^{x_0+nh} f(x)\,dx = h\int_0^n f(x_0+ph)\,dp$$

$$= h\int_0^n \left[f_0 + p\Delta f_0 + \frac{p(p-1)}{2!}\Delta^2 f_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 f_0 + \cdots\right]dp$$

[By Newton's forward interpolation formula]

$$= h\int_0^n \left[f_0 + p\Delta f_0 + \frac{1}{2}(p^2-p)\Delta^2 f_0 + \frac{1}{6}(p^3-3p^2+2p)\Delta^3 f_0 + \cdots\right]dp$$

$$= h\left[pf_0 + \frac{p^2}{2}\Delta f_0 + \frac{1}{2}\left(\frac{p^3}{3}-\frac{p^2}{2}\right)\Delta^2 f_0 + \frac{1}{6}\left(\frac{p^4}{4}-p^3+p^2\right)\Delta^3 f_0 + \cdots\right]_0^n$$

Hence,

$$\boxed{\int_{x_0}^{x_0+nh} f(x)\,dx = h\left[nf_0 + \frac{n^2}{2}\Delta f_0 + \frac{1}{2}\left(\frac{n^3}{3}-\frac{n^2}{2}\right)\Delta^2 f_0 + \frac{1}{6}\left(\frac{n^4}{4}-n^3+n^2\right)\Delta^3 f_0 + \cdots\right]} \quad (1)$$

which is the general quadrature formula, we obtain different quadrature formulae by taking $n = 1, 2, 3, \ldots$

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Trapezoidal Rule: Here the Integrand is approximated by a linear polynomial and integrated over the interval $x_0$ to $x_0+h$

$\therefore\ f(x) \simeq f_0 + p\,\Delta f_0$

Hence we get from equation (1)

$$\int_{x_0}^{x_0+h} f(x) = h\left[f_0 + \frac{1}{2}\Delta f_0\right] \qquad (\text{Put } n=1 \text{ upto II}^{nd} \text{ term})$$

$$= h\left[f_0 + \frac{1}{2}(f_1 - f_0)\right] = \frac{h}{2}\left[2f_0 + (f_1 - f_0)\right]$$

$$\Rightarrow \boxed{\int_{x_0}^{x_0+h} f(x)\,dx = \frac{h}{2}(f_0 + f_1)} \rightarrow \text{Basic Trapezoidal rule}$$

If we are to find $\int_a^b f(x)\,dx$ by trapezoidal rule then we divide interval $[a, b]$ into $n$ equal parts

$a = x_0,\ x_0+h,\ x_0+2h,\ \ldots,\ x_0+nh = b$ so that $h = \dfrac{b-a}{n}$

and apply trapezoidal rule in each subinterval as

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_0+nh} f(x)\,dx = \int_{x_0}^{x_0+h} f(x)\,dx + \int_{x_0+h}^{x_0+2h} f(x)\,dx + \cdots + \int_{x_0+(n-1)h}^{x_0+nh} f(x)\,dx.$$

$$= \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \cdots + \frac{h}{2}(f_{n-1} + f_n)$$

Hence,
$$\boxed{\int_a^b f(x)\,dx = \frac{h}{2}\left[f_0 + 2(f_1 + f_2 + \cdots + f_{n-1}) + f_n\right]} \rightarrow \text{Composite Trapezoidal rule}$$

Simpson's one third rule: Here the integrand is approximated by a quadratic polynomial and integrated over the interval $x_0$ to $x_0+2h$.

$\therefore\ f(x) \simeq f_0 + p\Delta f_0 + \frac{p(p-1)}{2}\Delta^2 f_0$

Hence, we get from equation (1),

$$\int_{x_0}^{x_0+2h} f(x)\,dx = h\left[2f_0 + 2\Delta f_0 + \frac{1}{3}\Delta^2 f_0\right] \quad \text{(Put } n=2 \text{ upto III term)}$$

$$= \frac{h}{3}\left[6f_0 + 6\Delta f_0 + \Delta^2 f_0\right]$$

$$= \frac{h}{3}\left[6f_0 + 6(f_1 - f_0) + (f_2 - 2f_1 + f_0)\right]$$

$$\left[\because \Delta^2 f_0 = (E-1)^2 f_0 = (E^2 - 2E + 1) f_0 = f_2 - 2f_1 + f_0\right]$$

$$\Rightarrow \boxed{\int_{x_0}^{x_0+2h} f(x)\,dx = \frac{h}{3}\left(f_0 + 4f_1 + f_2\right)} \rightarrow \text{Basic Simpson's rule}$$

and if interval $[a, b]$ is divided into $n$ equal parts such that $n$ is even, then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_0+nh} f(x)\,dx$$

$$= \int_{x_0}^{x_0+2h} f(x)\,dx + \int_{x_0+2h}^{x_0+4h} f(x)\,dx + \int_{x_0+4h}^{x_0+6h} f(x)\,dx + \cdots + \int_{x_0+(n-2)h}^{x_0+nh} f(x)\,dx$$

$$= \frac{h}{3}\left(f_0 + 4f_1 + f_2\right) + \frac{h}{3}\left(f_2 + 4f_3 + f_4\right) + \cdots + \frac{h}{3}\left(f_{n-2} + 4f_{n-1} + f_n\right)$$

$$\Rightarrow \boxed{\int_a^b f(x)\,dx = \frac{h}{3}\left[f_0 + 4(f_1 + f_3 + f_5 + \cdots + f_{n-1}) + 2(f_2 + f_4 + \cdots + f_{n-2}) + f_n\right]}$$

Composite Simpson's rule

Simpson's Three-eight rule: Here the integrand is approximated by a cubic polynomial and integrated over the interval $x_0$ to $x_0 + 3h$.

$$\therefore f(x) \simeq f_0 + p\Delta f_0 + \frac{p(p-1)}{2}\Delta^2 f_0 + \frac{p(p-1)(p-2)}{6}\Delta^3 f_0$$

Hence, we get from equation (1),

$$\int_{x_0}^{x_0+3h} f(x)\,dx = h\left[3f_0 + \frac{9}{2}\Delta f_0 + \frac{1}{2}\left(9-\frac{9}{2}\right)\Delta^2 f_0 + \frac{1}{6}\left(\frac{81}{4}-27+9\right)\Delta^3 f_0\right]$$

(Put $n=3$ upto $IV^{th}$ term)

$$= h\left[3f_0 + \frac{9}{2}(f_1-f_0) + \frac{9}{4}(f_2-2f_1+f_0) + \frac{3}{8}(f_3-3f_2+3f_1-f_0)\right]$$

$$\Rightarrow \boxed{\int_{x_0}^{x_0+3h} f(x)\,dx = \frac{3h}{8}\left[f_0+3f_1+3f_2+f_3\right]} \rightarrow \text{Basic Simpson } \tfrac{3}{8} \text{ rule}$$

and if interval $[a,b]$ is divided into $n$ equal parts such that $n$ is multiple of 3, then

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_0+nh} f(x)\,dx$$

$$= \int_{x_0}^{x_0+3h} f(x)\,dx + \int_{x_0+3h}^{x_0+6h} f(x)\,dx + \cdots + \int_{x_0+(n-3)h}^{x_0+nh} f(x)\,dx$$

$$= \frac{3h}{8}\left[f_0+3f_1+3f_2+f_3\right] + \frac{3h}{8}\left[f_3+3f_4+3f_5+f_6\right] + \cdots + \frac{3h}{8}\left[f_{n-3}+3f_{n-2}+3f_{n-1}+f_n\right]$$

$$\Rightarrow \boxed{\int_a^b f(x)\,dx = \frac{3h}{8}\left[f_0 + 3(f_1+f_2+f_4+f_5+\cdots+f_{n-2}+f_{n-1}) + 2(f_3+f_6+\cdots+f_{n-3}) + f_n\right]}$$

This is known as Composite Simpson $\frac{3}{8}$ rule.

Que Compute $\int_0^1 \frac{\sin x}{x}\, dx$ by using the composite trapezoid rule with 6 uniform points.

Sol Here $x_0 = 0$, $x_n = x_0 + nh = 1$, $n = 5$ ($\because$ we have to take 6 uniform points)

$\therefore$ $0 + 5h = 1 \Rightarrow h = \frac{1}{5} = 0.2$

| $x$ | $f(x) = \frac{\sin x}{x}$ |
|---|---|
| $x_0 = 0.0$ | 1.00000 |
| $x_1 = 0.2$ | 0.99335 |
| $x_2 = 0.4$ | 0.97355 |
| $x_3 = 0.6$ | 0.94107 |
| $x_4 = 0.8$ | 0.89670 |
| $x_5 = 1.0$ | 0.84147 |

(we have assigned $\frac{\sin x}{x} = 1$ at $x = 0$ $\because \lim_{x \to 0} \frac{\sin x}{x} = 1$)

$\therefore$ By trapezoidal rule,

$$\int_0^1 \frac{\sin x}{x}\, dx = \frac{h}{2}\left[f_0 + 2(f_1 + f_2 + f_3 + f_4) + f_5\right]$$

$$= \frac{0.2}{2}\left[1.00000 + 2(0.99335 + 0.97355 + 0.94107 + 0.89670) + 0.84147\right]$$

$$= 0.94508 \quad \text{Ans}$$

Que Using the basic Trapezoid Rule and the basic Simpson's Rule, find approximate values for the integral

$$\int_0^1 e^{-x^2}\, dx$$

**Sol** Here $x_0 = 0$, $x_n = 1$, $f(x) = e^{-x^2}$

**For Basic Trapezoid Rule** Here $x_0 = 0$, $x_1 = 1$, $h = 1$

$$\int_0^1 e^{-x^2}dx = \frac{h}{2}[f_0 + f_1]$$

$$= \frac{1}{2}[e^0 + e^{-1}]$$

$$= 0.5[1 + 0.36788] = 0.68394$$

**For Basic Simpson's Rule**

Here $x_0 = 0$, $x_1 = 0.5$, $x_2 = 1$, $h = 0.5$

$$\int_0^1 e^{-x^2}dx = \frac{h}{3}[f_0 + 4f_1 + f_2]$$

$$= \frac{0.5}{3}[e^0 + 4e^{-0.25} + e^{-1}]$$

$$= 0.16667[1 + 4(0.77880) + 0.36788] = 0.7472$$

**Que:** A train is moving at the speed of 30m/sec. Suddenly brakes are applied. The speed of the train per second after $t$ seconds is given by

| Time ($t$) | 0 | 5 | 10 | 15 | 20 | 25 | 30 | 35 | 40 | 45 |
|---|---|---|---|---|---|---|---|---|---|---|
| Speed ($v$) | 30 | 24 | 19 | 16 | 13 | 11 | 10 | 8 | 7 | 5 |
| | 1 | 3 | 3 | 1+1 | 3 | 3 | 1+1 | 3 | 3 | 1 |

Apply Simpson's three-eighth rule to determine the distance moved by the train in 45 seconds.

**Sol** If $s$ metres is the distance covered in $t$ seconds, then

$$\frac{ds}{dt} = v$$

$$\Rightarrow ds = v\,dt \Rightarrow \int_{t=0}^{45} ds = \int_0^{45} v\,dt$$

$$\Rightarrow [s]_{t=0}^{t=45} = \int_0^{45} v\,dt$$

Here $x_0 = 0$, $h = 5$, $x_0 + nh = 45$

$\Rightarrow 0 + 5n = 45 \Rightarrow n = 9$ which is multiple of 3.

$\therefore$ By Simpson's three-eighth rule,

$$\int_0^{45} v\,dt = \frac{3h}{8}\left[V_0 + 3(V_1 + V_2 + V_4 + V_5 + V_7 + V_8) + 2(V_3 + V_6) + V_9\right]$$

$\Rightarrow$ The distance moved in 45 seconds

$$= \frac{3\times5}{8}\left[30 + 3(24+19+13+11+8+7) + 2(16+10) + 5\right]$$

$$= \frac{15}{8}\left[30 + 246 + 52 + 5\right] = \frac{15}{8}\times 333 = 624.375 \text{ metres}$$

Ans

**Que** Find the approximate value of $\pi$ by calculating to 4 decimal places from $\int_0^1 \frac{1}{(1+x^2)}\,dx$ using
(i) Trapezoidal rule
(ii) Simpson $\frac{1}{3}$ rule
(iii) Simpson $\frac{3}{8}$ rule

by taking $n = 12$.

**Sol** Given $x_0 = 0$, $n = 12$, $x_0 + nh = 1 \Rightarrow 0 + 12h = 1 \Rightarrow h = \frac{1}{12}$

$\therefore$ We have

| $x$ | $f(x) = \frac{1}{(1+x^2)}$ |
|---|---|
| 0 | $1 = f_0$ |
| 1/12 | $144/145 = 0.993103 = f_1$ |
| 2/12 = 1/6 | $36/37 = 0.972973 = f_2$ |
| 3/12 = 1/4 | $16/17 = 0.941176 = f_3$ |
| 4/12 = 1/3 | $9/10 = 0.9 = f_4$ |
| 5/12 | $144/169 = 0.852071 = f_5$ |
| 6/12 = 1/2 | $4/5 = 0.8 = f_6$ |
| 7/12 | $144/193 = 0.746114 = f_7$ |
| 8/12 = 2/3 | $9/13 = 0.692308 = f_8$ |
| 9/12 = 3/4 | $16/25 = 0.64 = f_9$ |
| 10/12 = 5/6 | $36/61 = 0.590164 = f_{10}$ |
| 11/12 | $144/265 = 0.543396 = f_{11}$ |
| 12/12 = 1 | $1/2 = 0.5 = f_{12}$ |

Exact value of $\int_0^1 \frac{1}{(1+x^2)}\,dx = (\tan^{-1}x)_0^1 = \frac{\pi}{4}$

(i) By Trapezoidal rule

$$\int_0^1 \frac{1}{(1+x^2)}\,dx = \frac{h}{2}\left[f_0+2(f_1+f_2+\cdots+f_{11})+f_{12}\right]$$

$$= \frac{1}{24}\left[1+2\times 8.671305+0.5\right] = \frac{1}{24}\times 18.84261 = 0.78510875$$

$\Rightarrow \frac{\pi}{4} \simeq 0.78510875$

$\Rightarrow$ Approximate value of $\pi \simeq 3.14043$ (by trapezoidal rule)

(ii) By Simpson $\frac{1}{3}$ rule

$$\int_0^1 \frac{1}{(1+x^2)}\,dx = \frac{h}{3}\left[f_0+4(f_1+f_3+f_5+f_7+f_9+f_{11})+2(f_2+f_4+f_6+f_8+f_{10}) + f_{12}\right]$$

$$= \frac{1}{36}\left[1+4\times 4.71586+2\times 3.955445+0.5\right]$$

$$= \frac{1}{36}\times 28.27433 = 0.785398056$$

$\Rightarrow \frac{\pi}{4} \simeq 0.785398056$

$\Rightarrow$ Approximate value of $\pi \simeq 3.1416$ (by Simpson $\frac{1}{3}$ rule)

(iii) By Simpson $\frac{3}{8}$ rule

$$\int_0^1 \frac{1}{(1+x^2)}\,dx = \frac{3h}{8}\left[f_0+3(f_1+f_2+f_4+f_5+f_7+f_8+f_{10}+f_{11}) + 2(f_3+f_6+f_9)+f_{12}\right]$$

$$= \frac{1}{32}\left[1+3(6.290129)+2(2.381176)+0.5\right]$$

$$= \frac{1}{32}\times 25.132739 = 0.785398094$$

$\Rightarrow \frac{\pi}{4} \simeq 0.785398094$

$\Rightarrow$ Approximate value of $\pi \simeq 3.1416$ (by Simpson $\frac{3}{8}$ rule)

# Errors in Quadrature Formulae:

## Error Term in Trapezoidal Rule:

In trapezoidal rule, we approximate

$$\int_{x_0}^{x_0+h} f(x)\,dx \quad \text{by} \quad \frac{h}{2}\left[f(x_0)+f(x_0+h)\right]$$

$$\therefore \text{Error} = \int_{x_0}^{x_0+h} f(x)\,dx - \frac{h}{2}\left[f(x_0)+f(x_0+h)\right]$$

Let $f(x) = F'(x)$

$$\therefore \text{Error} = F(x_0+h) - F(x_0) - \frac{h}{2}\left[f(x_0)+f(x_0+h)\right]$$

$$= \left\{\cancel{F(x_0)} + hF'(x_0) + \frac{h^2}{2!}F''(x_0) + \frac{h^3}{3!}F'''(x_0) + \cdots\right\}$$

$$- \cancel{F(x_0)} - \frac{h}{2}f(x_0) - \frac{h}{2}\left\{f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \frac{h^3}{3!}f'''(x_0) + \cdots\right\}$$

(by Taylor's series)

$$= \left\{\cancel{hf(x_0)} + \frac{h^2}{2}f'(x_0) + \frac{h^3}{6}f''(x_0) + \cdots\right\} - \cancel{hf(x_0)} - \frac{h^2}{2}f'(x_0) - \frac{h^3}{4}f''(x_0) - \frac{h^4}{12}f'''(x_0) + \cdots$$

$(\because F'(x) = f(x))$

$$= -\frac{h^3}{12}f''(x_0) + \cdots$$

$$\therefore \boxed{\text{Error} = -\frac{h^3}{12}f''(\xi)}$$ where $\xi$ is any point lying between $x_0$ & $x_0+h$

If we are to find $\int_a^b f(x)\,dx$ and $[a,b]$ is divided into $n$ subintervals at $a = x_0, x_0+h, \ldots, x_0+nh = b$, then

$$\text{Error} = -\frac{h^3}{12}\left[f''(\xi_1) + f''(\xi_2) + \cdots + f''(\xi_n)\right] \quad \text{where } x_{i-1} < \xi_i < x_i$$

$$= -\frac{nh^3}{12}\left[\frac{f''(\xi_1)+f''(\xi_2)+\cdots+f''(\xi_n)}{n}\right] = -\frac{nh^3}{12}f''(\xi)$$

where $a < \xi < b$

($\because$ The average $\frac{1}{n}\sum_{i=1}^{n} f''(\xi_i)$ lies between the least and greatest values of $f''$ on the interval $(a,b)$. So, by intermediate-value theorem it is $f''(\xi)$)

for some $\xi$ in $(a,b)$)

Hence, $$\boxed{\text{Error} = -\frac{(b-a)h^2 f''(\xi)}{12}}$$ $\because nh = b-a$

for some $\xi$ in $(a,b)$.

$\therefore$ Error is of order two.

<u>Note:</u> In the above discussion, we have applied the following Intermediate-Value Theorem: If the function $g$ is continuous on an interval $[a,b]$, then for each $c$ between $g(a)$ and $g(b)$, there is a point $\xi$ in $(a,b)$ for which $g(\xi) = c$.

## Error Term in Simpson's One-third rule:

In Simpson's $\frac{1}{3}$ rule, we approximate

$$\int_{x_0}^{x_0+2h} f(x)\,dx \text{ by } \frac{h}{3}\left[f(x_0)+4f(x_0+h)+f(x_0+2h)\right]$$

$$\therefore \text{Error} = \int_{x_0}^{x_0+2h} f(x)\,dx - \frac{h}{3}\left[f(x_0)+4f(x_0+h)+f(x_0+2h)\right]$$

Let $f(x) = F'(x)$

$$\therefore \text{Error} = F(x_0+2h) - F(x_0) - \frac{h}{3}\left[f(x_0)+4f(x_0+h)+f(x_0+2h)\right]$$

$$= \left\{ \cancel{F(x_0)} + 2hF'(x_0) + \frac{(2h)^2}{2!}F''(x_0) + \frac{(2h)^3}{3!}F'''(x_0) + \frac{(2h)^4}{4!}F^{IV}(x_0) + \frac{(2h)^5}{5!}F^{V}(x_0) + \cdots \right\} - \cancel{F(x_0)} - \frac{h}{3}f(x_0)$$

$$-\frac{4h}{3}\left\{f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \frac{h^3}{3!}f'''(x_0) + \frac{h^4}{4!}f^{IV}(x_0) + \cdots\right\}$$

$$-\frac{h}{3}\left\{f(x_0) + 2hf'(x_0) + \frac{(2h)^2}{2!}f''(x_0) + \frac{(2h)^3}{3!}f'''(x_0) + \frac{(2h)^4}{4!}f^{IV}(x_0) + \cdots\right\}$$

(by Taylor's series)

$$= \cancel{2hf(x_0)} + \cancel{2h^2f'(x_0)} + \cancel{\frac{4}{3}h^3f''(x_0)} + \frac{2}{3}h^4f'''(x_0) + \frac{4}{15}h^5f^{IV}(x_0) + \cdots$$

$$- \cancel{2hf(x_0)} - \cancel{2h^2f'(x_0)} - \cancel{\frac{4}{3}h^3f''(x_0)} - \left(\frac{2}{9}+\frac{4}{9}\right)h^4f'''(x_0) - \left(\frac{1}{18}+\frac{2}{9}\right)h^5f^{IV}(x_0) + \cdots$$

$(\because F'(x) = f(x))$

$$= \left(\frac{4}{15} - \frac{5}{18}\right)h^5f^{IV}(x_0) + \cdots$$

$$= -\frac{h^5}{90}f^{IV}(x_0) + \cdots$$

$\therefore$ $\boxed{\text{Error} = -\frac{h^5}{90}f^{IV}(\xi)}$ where $\xi$ is any point between $x_0$ and $x_0+2h$.

If we are to find $\int_a^b f(x)\,dx$ and $[a,b]$ is divided into $n$ subintervals where $n$ is even at $a = x_0, x_0+h, \ldots, x_0+nh = b$, then

$$\text{Error} = -\frac{h^5}{90}\left[f^{IV}(\xi_1) + f^{IV}(\xi_2) + \cdots + f^{IV}(\xi_{n/2})\right] \text{ where } x_{2i-2} < \xi_i < x_{2i}$$

$$= -\frac{nh^5}{180}\left[\frac{f^{IV}(\xi_1) + f^{IV}(\xi_2) + \cdots + f^{IV}(\xi_{n/2})}{n/2}\right]$$

$$= -\frac{nh^5}{180}f^{iv}(\xi) \quad \text{where } a < \xi < b \quad (\text{as above})$$

$\therefore$ $\boxed{\text{Error} = -\frac{(b-a)h^4}{180}f^{(4)}(\xi)}$ $(\because nh = b-a)$

where $a < \xi < b$

Hence, error in Simpson's one-third rule is of order 4.

Note: Simpson's one-third rule is simply known as Simpson's Rule.

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## Error Term in Simpson's Three-Eight Rule:

In Simpson's $\frac{3}{8}$ rule, we approximate

$$\int_{x_0}^{x_0+3h} f(x)\,dx \text{ by } \frac{3h}{8}\left[f(x_0)+3f(x_0+h)+3f(x_0+2h)+f(x_0+3h)\right]$$

$$\therefore \text{Error} = \int_{x_0}^{x_0+3h} f(x)\,dx - \frac{3h}{8}\left[f(x_0)+3f(x_0+h)+3f(x_0+2h)+f(x_0+3h)\right]$$

Let $f(x) = F'(x)$

$$\therefore \text{Error} = F(x_0+3h)-F(x_0)-\frac{3h}{8}\left[f(x_0)+3f(x_0+h)+3f(x_0+2h)+f(x_0+3h)\right]$$

$$= \Big\{\cancel{F(x_0)}+3hF'(x_0)+\frac{9h^2}{2!}F''(x_0)+\frac{27h^3}{3!}F'''(x_0)+\frac{81h^4}{4!}F^{(4)}(x_0)$$

$$+\frac{243h^5}{5!}F^{(5)}(x_0)+\frac{729h^6}{6!}F^{(6)}(x_0)+\cdots\Big\}-\cancel{F(x_0)}$$

$$-\frac{3h}{8}\Big[f(x_0)+3\Big\{f(x_0)+hf'(x_0)+\frac{h^2}{2!}f''(x_0)+\frac{h^3}{3!}f'''(x_0)+\frac{h^4}{4!}f^{(4)}(x_0)$$

$$+\frac{h^5}{5!}f^{(5)}(x_0)+\cdots\Big\}+3\Big\{f(x_0)+2hf'(x_0)+2h^2f''(x_0)+\frac{4h^3}{3}f'''(x_0)$$

$$+\frac{2}{3}h^4f^{(4)}(x_0)+\frac{4}{15}h^5f^{(5)}(x_0)+\cdots\Big\}+\Big\{f(x_0)+3hf'(x_0)+\frac{9h^2}{2}f''(x_0)$$

$$+\frac{9h^3}{2}f'''(x_0)+\frac{27}{8}h^4f^{(4)}(x_0)+\frac{81}{40}h^5f^{(5)}(x_0)+\cdots\Big\}\Big]$$

(by Taylor's series)

$$=\Big\{3hf(x_0)+\frac{9}{2}h^2f'(x_0)+\frac{9}{2}h^3f''(x_0)+\frac{27}{8}h^4f'''(x_0)+\frac{81h^5}{40}f^{(4)}(x_0)$$

$$+\frac{81h^6}{80}f^{(5)}(x_0)+\cdots\Big\}-\frac{3h}{8}\Big[8f(x_0)+12hf'(x_0)+12h^2f''(x_0)+9h^3f'''(x_0)$$

$$+\frac{11h^4}{2}f^{(4)}(x_0)+\cdots\Big] \qquad (\because F'(x)=f(x))$$

$$= -\frac{3}{80}h^5f^{(4)}(x_0)+\cdots$$

$$\therefore \boxed{\text{Error} = -\frac{3}{80}h^5f^{(4)}(\xi)} \quad \text{where } x_0<\xi<x_0+3h$$

If we are to find $\int_a^b f(x)\,dx$ and $[a,b]$ is divided into $n$ subintervals where $n$ is multiple of 3 at

$$a = x_0,\ x_0+h, \ldots, x_0+nh = b, \text{ then}$$

$$\text{Error} = -\frac{3}{80}h^5\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_2) + \cdots + f^{(4)}(\xi_{n/3})\right]$$

where $x_{3i-3} < \xi_i < x_{3i}$

$$= -\frac{nh^5}{80}\left[\frac{f^{(4)}(\xi_1) + f^{(4)}(\xi_2) + \cdots + f^{(4)}(\xi_{n/3})}{n/3}\right]$$

$$= -\frac{nh^5}{80} f^{(4)}(\xi) \quad \text{where } a < \xi < b \qquad \text{(as above)}$$

$$\therefore \boxed{\text{Error} = -\frac{(b-a)h^4 f^{(4)}(\xi)}{80}} \qquad (\because nh = b-a)$$

where $a < \xi < b$

Hence, error in Simpson's three-eight rule is of order 4.

<u>Que</u> If the composite trapezoid rule is to be used to compute

$$\int_0^1 e^{-x^2}\,dx$$

with an error of at most $\frac{1}{2}\times 10^{-4}$, how many points should be used?

<u>Sol</u> The error formula is $-\frac{(b-a)}{12}h^2 f''(\xi)$ where $0 < \xi < 1$

In this example, $f(x) = e^{-x^2}$, $f'(x) = -2xe^{-x^2}$ and $f''(x) = (4x^2-2)e^{-x^2}$.

Thus, $|f''(x)| \leq 2$ on the interval $[0,1]$, $a=0, b=1$

Now, $|\text{error}| \leq \frac{1}{12}h^2 \times 2 = \frac{h^2}{6}$

$\therefore$ To have an error of at most $\frac{1}{2}\times 10^{-4}$, we require

$\frac{1}{6}h^2 \leq \frac{1}{2}\times 10^{-4}$ or $h \leq 0.01732$

In this example, $h = \frac{1}{n}$ $\quad (\because \; nh = b-a = 1)$

$\therefore \quad \frac{1}{n} \leq 0.01732 \Rightarrow n \geq 58$

Hence, 59 or more points should be used.

## Romberg Algorithm:

The Romberg algorithm produces a triangular array of numbers, all of which are numerical estimates of the definite integral $\int_a^b f(x)\,dx$. The array is denoted here by the notation

$$
\begin{array}{lllll}
R(0,0) & & & & \\
R(1,0) & R(1,1) & & & \\
R(2,0) & R(2,1) & R(2,2) & & \\
R(3,0) & R(3,1) & R(3,2) & R(3,3) & \\
\vdots & \vdots & \vdots & \vdots & \ddots \\
R(n,0) & R(n,1) & R(n,2) & R(n,3) & \cdots\ R(n,n)
\end{array}
$$

The first column of this table contains estimates of the integral obtained by the recursive trapezoid formula with decreasing values of the step size. Explicitly, $R(n,0)$, is the result of applying the trapezoid rule with $2^n$ equal subintervals. The first of them $R(0,0)$, is obtained with just one trapezoid:

$$R(0,0) = \frac{(b-a)}{2}\left[f(a) + f(b)\right]$$

By using the recursive trapezoid rule, we find that the first column of the Romberg algorithm is

$$R(n,0) = \frac{1}{2}R(n-1,0) + h\sum_{k=1}^{2^{n-1}} f\left[a + (2k-1)h\right] \quad \text{——— (1)}$$

where $h = \dfrac{b-a}{2^n}$ and $n \geqslant 1$.

The second and successive columns in the Romberg array are generated by the Richardson extrapolation formula

$$R(n,m) = R(n,m-1) + \frac{1}{4^m-1}\left[R(n,m-1) - R(n-1,m-1)\right] \quad \text{--- (2)}$$

with $n \geq 1$ and $m \geq 1$.

The error is $O(h^2)$ for the first column,
$O(h^4)$ for the second column,
$O(h^6)$ for the third column, and so on.

Que If $R(4,2) = 8$ and $R(3,2) = 1$, what is $R(4,3)$?

Sol From equation (2), we have

$$R(4,3) = R(4,2) + \frac{1}{63}\left[R(4,2) - R(3,2)\right]$$

$$= 8 + \frac{1}{63}(8-1) = 8 + \frac{1}{9} = \frac{73}{9} \quad \text{Ans}$$

Que By the Romberg algorithm, approximate $\int_0^2 \frac{4}{(1+x^2)}\,dx$ by evaluating $R(1,1)$.

Sol Here $a = 0$, $b = 2$, $f(x) = \frac{4}{(1+x^2)}$

$$\therefore R(0,0) = \frac{(b-a)}{2}\left[f(a) + f(b)\right] = 1.\left[4 + \frac{4}{5}\right] = \frac{24}{5}$$

Now, $R(1,0) = \frac{1}{2}R(0,0) + h\,f(a+h)$ (by equ. (1) $\because n = 1$)

where $h = \frac{b-a}{2} = \frac{2}{2} = 1$

$$\therefore R(1,0) = \frac{1}{2} \times \frac{24}{5} + 1.f(1) = \frac{12}{5} + 1 \times \frac{4}{2} = \frac{12}{5} + 2 = \frac{22}{5}$$

Hence $R(1,1) = R(1,0) + \frac{1}{3}\left[R(1,0) - R(0,0)\right]$

$$= \frac{22}{5} + \frac{1}{3}\left[\frac{22}{5} - \frac{24}{5}\right] = \frac{22}{5} - \frac{2}{15} = \frac{66-2}{15} = \frac{64}{15} = 4.267 \quad \text{Ans}$$

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**Que** Evaluate $\int_0^1 \frac{dx}{1+x}$ correct to three decimal places using Romberg's method. Hence find the value of $\log_e 2$.

**Sol** Here $a=0,\ b=1,\ f(x)=\frac{1}{1+x}$

$$\therefore R(0,0) = \frac{(b-a)}{2}[f(a)+f(b)] = \frac{(1-0)}{2}[f(0)+f(1)]$$
$$= \frac{1}{2}\left[1+\frac{1}{2}\right] = \frac{3}{4} = 0.75$$

Now, we know that first column of the Romberg algorithm is given by $R(n,0) = \frac{1}{2}R(n-1,0) + h\sum_{k=1}^{2^{n-1}} f[a+(2k-1)h]$ —— (2)

where $h = \frac{b-a}{2^n}$ and $n \geq 1$.

and the successive columns in the Romberg array are generated by $R(n,m) = R(n,m-1) + \frac{1}{4^m-1}[R(n,m-1) - R(n-1,m-1)]$ —— (3)

with $n \geq 1$ and $m \geq 1$

$\therefore$ By equ. (2), $R(1,0) = \frac{1}{2}R(0,0) + \frac{b-a}{2}\sum_{k=1}^{1} f[a+(2k-1)h]$

$$= \frac{1}{2}\times 0.75 + \frac{1-0}{2} f(a+h) \qquad h = \frac{b-a}{2}$$

$$= \frac{1}{2}\times 0.75 + \frac{1}{2}\times\frac{1}{1+1/2} \qquad h = \frac{1-0}{2} = \frac{1}{2}$$

$$= 0.375 + \frac{1}{3} = 0.375 + 0.33333 = 0.70833$$

$\therefore$ By equ.(3),

$$R(1,1) = R(1,0) + \frac{1}{3}[R(1,0) - R(0,0)]$$

$$\therefore R(1,1) = 0.70833 + \frac{1}{3}[0.70833 - 0.75] = 0.69444$$

By equ. (2), $R(2,0) = \frac{1}{2}R(1,0) + h\sum_{k=1}^{2} f[0+(2k-1)h]$ where $h = \frac{b-a}{2^2} = \frac{1}{4}$

$$\therefore R(2,0) = \frac{1}{2}\times 0.70833 + \frac{1}{4}[f(h)+f(3h)] \quad (\text{by equ } (2))$$

$$= \frac{1}{2}\times 0.70833 + \frac{1}{4}\left[f\left(\frac{1}{4}\right) + f\left(\frac{3}{4}\right)\right]$$

$$= 0.354165 + \frac{1}{4}\left[\frac{1}{1+\frac{1}{4}} + \frac{1}{1+\frac{3}{4}}\right]$$

$$= 0.354165 + \left[\frac{1}{5} + \frac{1}{7}\right] = 0.354165 + 0.2 + 0.142857$$

$$= 0.69702$$

Now, by equ. (3),

$$R(2,1) = R(2,0) + \frac{1}{3}\left[R(2,0) - R(1,0)\right]$$

$$= 0.69702 + \frac{1}{3}\left[0.69702 - 0.70833\right]$$

$$= \frac{4}{3}\times 0.69702 - \frac{1}{3}\times 0.70833 = 0.69325$$

Now, again by equ. (3),

$$R(2,2) = R(2,1) + \frac{1}{15}\left[R(2,1) - R(1,1)\right]$$

$$= 0.69325 + \frac{1}{15}\left[0.69325 - 0.69444\right] = 0.69317$$

Hence the value of the integral

$$\int_0^1 \frac{dx}{(1+x)} = 0.693 \quad (\text{correct to 3D}) \quad \text{———} (4)$$

$$\text{Also,} \quad \int_0^1 \frac{dx}{(1+x)} = \left| \log(1+x) \right|_0^1 = \log_e 2 \quad \text{———} (5)$$

Hence from (4) and (5),

$$\log_e 2 = 0.693$$

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## Gaussian Quadrature Formulas

Description Most numerical integration formulas conform to the following pattern:

$$\int_a^b f(x)\,dx \approx A_0 f(x_0) + A_1 f(x_1) + \cdots + A_n f(x_n)$$

To use such a formula it is necessary only to know the nodes $x_0, x_1, \ldots, x_n$ and the weights $A_0, A_1, \ldots, A_n$.

If the nodes have been fixed, then there is a corresponding Lagrange interpolation formula:

$$p(x) = \sum_{i=0}^{n} l_i(x) f(x_i) \quad \text{where } l_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \left(\frac{x-x_j}{x_i-x_j}\right)$$

This formula provides a polynomial $p$ of degree at most $n$ that interpolates $f$ at the nodes i.e, $p(x_i) = f(x_i)$ for $0 \le i \le n$. When the circumstances are favourable, $p$ is a good approximation to $f$. Therefore, we obtain

$$\int_a^b f(x)\,dx \approx \int_a^b p(x)\,dx = \sum_{i=0}^{n} f(x_i)\left\{\int_a^b l_i(x)\,dx\right\}$$

$$= \sum_{i=0}^{n} A_i f(x_i)$$

where $A_i = \int_a^b l_i(x)\,dx$

This formula gives correct values for the integral of every polynomial of degree at most $n$.

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**Que** Find the quadrature formula

$$\int_{-2}^{2} f(x)\,dx \approx A_0 f(-1) + A_1 f(0) + A_2 f(1)$$

i.e, nodes are $-1, 0, 1$ and the interval is $[-2, 2]$.

**Sol** We have $A_i = \int_a^b l_i(x)\,dx$ where $l_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \left(\frac{x - x_j}{x_i - x_j}\right)$

Here $a = -2$, $b = 2$, $x_0 = -1$, $x_1 = 0$, $x_2 = 1$

$$\therefore\ l_0(x) = \frac{x(x-1)}{(-1)(-1-1)} = \frac{1}{2}x(x-1) = \frac{1}{2}(x^2 - x)$$

$$l_1(x) = \frac{(x+1)(x-1)}{(0+1)(0-1)} = -(x^2-1) = 1 - x^2$$

$$l_2(x) = \frac{(x+1)(x-0)}{(1+1)(1-0)} = \frac{x(x+1)}{2} = \frac{1}{2}(x^2 + x)$$

$$\therefore\ A_0 = \int_{-2}^{2} \frac{1}{2}(x^2 - x)\,dx = \int_0^2 x^2\,dx = \left(\frac{x^3}{3}\right)_0^2 = \frac{8}{3}$$

$\left(\because \int_{-2}^{2} x\,dx = 0 \text{ being an odd function}\right)$

$$A_1 = \int_{-2}^{2} (1 - x^2)\,dx = 2\left(x - \frac{x^3}{3}\right)_0^2 = 2\left(2 - \frac{8}{3}\right) = -\frac{4}{3}$$

(even function)

$$A_2 = \int_{-2}^{2} \frac{1}{2}(x^2 + x)\,dx = \frac{2}{2}\int_0^2 x^2\,dx = \frac{8}{3}$$

$\left(\because \int_{-2}^{2} x\,dx = 0\right)$

$\therefore$ The quadrature formula is

$$\int_{-2}^{2} f(x)\,dx \approx \frac{8}{3} f(-1) - \frac{4}{3} f(0) + \frac{8}{3} f(1)$$

**Note:** The above formula provides correct values for any quadratic polynomial.

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## Gausian Quadrature Theorem:

Let $q$ be a nontrivial polynomial of degree $n+1$ such that $\int_a^b x^k q(x)\,dx = 0 \quad (0 \le k \le n)$

Let $x_0, x_1, \ldots, x_n$ be the zeros of $q$. Then the formula

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i) \quad \text{where } A_i = \int_a^b l_i(x)\,dx \quad \text{—— (1)}$$

with these $x_i$'s as nodes will be exact for all polynomials of degree at most $2n+1$. Furthermore, the nodes lie in the open interval.

$$\left(\text{Here } l_i(x) = \prod_{\substack{j=0\\ j\neq i}}^{n} \left(\frac{x-x_j}{x_i-x_j}\right)\right)$$

Proof: Let $f$ be any polynomial of degree $\le 2n+1$. Dividing $f$ by $q$, we obtain a quotient $p$ and a remainder $r$, both of which have degree at most $n$:

$$f = pq + r$$

By our hypothesis $\int_a^b p(x)\,q(x)\,dx = 0$

$$\therefore \int_a^b f(x)\,dx = \int_a^b r(x)\,dx \qquad (\because f(x_i) = p(x_i)q(x_i) + r(x_i) = r(x_i))$$

$(\because x_i \text{ is a root of } q)$

$$= \sum_{i=0}^{n} A_i r(x_i) \qquad \text{where } A_i = \int_a^b l_i(x)\,dx$$

$$= \sum_{i=0}^{n} A_i f(x_i)$$

Note: With arbitrary nodes, Formula (1) is exact for all polynomial of degree $\le n$. With the Gaussian nodes, Formula (1) is exact for all polynomial of degree $\le 2n+1$.

The quadrature formula that arise as applications of this theorem are called Gaussian quadrature rules.

Que Determine the Gaussian quadrature formula with three Gaussian nodes and three ~~root~~ weights for the integral $\int_{-1}^{1} f(x)\,dx$

Sol By Gaussian quadrature Theorem, degree of $q$ is 3, so $q$ is of the form

$$q(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3$$

and satisfy $\int_{-1}^{1} q(x)\,dx = \int_{-1}^{1} x\,q(x)\,dx = \int_{-1}^{1} x^2 q(x)\,dx = 0$

If we let $c_0 = c_2 = 0$, then $q(x) = c_1 x + c_3 x^3$ and so

$$\int_{-1}^{1} q(x)\,dx = \int_{-1}^{1} x^2 q(x)\,dx = 0 \qquad (\because \text{ both are odd-functions})$$

To obtain $c_1$ and $c_3$, we impose the condition

$$\int_{-1}^{1} x\,(c_1 x + c_3 x^3)\,dx = 0$$

$$\Rightarrow \quad 2\int_{0}^{1} x\,(c_1 x + c_3 x^3)\,dx = 0$$

$$\Rightarrow \quad \frac{c_1}{3} + \frac{c_3}{5} = 0 \Rightarrow 5c_1 + 3c_3 = 0 \Rightarrow \frac{c_1}{c_3} = \frac{-3}{5}$$

$\therefore$ We can choose $c_1 = -3$, $c_3 = 5$ (or any multiple of that)

$\therefore \; q(x) = -3x + 5x^3$

$q(x) = 0$ when $x(5x^2 - 3) = 0 \Rightarrow x = 0, \pm\sqrt{\frac{3}{5}}$

which are the Gaussian nodes for the desired quadrature formula.

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Now, we want to obtain the weights $A_0$, $A_1$ and $A_2$ in the formula

$$\int_{-1}^{1} f(x)\,dx \approx A_0 f\left(-\sqrt{\tfrac{3}{5}}\right) + A_1 f(0) + A_2 f\left(\sqrt{\tfrac{3}{5}}\right) \quad \text{—(1)}$$

so that the approximate equality($\approx$) is an exact equality ($=$) whenever $f$ is of the form $ax^2+bx+c$.

Now, formula (1) is exact for all polynomials of degree $\leq 2$ if it is exact for these three monomials: $1$, $x$, and $x^2$.

$\therefore$ from equ.(1),

$$\int_{-1}^{1} 1\,dx = 2 = A_0 + A_1 + A_2$$

$$\int_{-1}^{1} x\,dx = 0 = -\sqrt{\tfrac{3}{5}}\,A_0 + \sqrt{\tfrac{3}{5}}\,A_2$$

$$\int_{-1}^{1} x^2\,dx = \frac{2}{3} = \frac{3}{5}A_0 + \frac{3}{5}A_2$$

Solving these we get $A_0 = A_2 = \frac{5}{9}$ and $A_1 = \frac{8}{9}$

$\therefore$ The final formula is

$$\boxed{\int_{-1}^{1} f(x)\,dx \approx \frac{5}{9} f\left(-\sqrt{\tfrac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\tfrac{3}{5}}\right)} \quad \text{—(2)}$$

which integrate correctly all polynomials up to and including quintic ones.

Change of Intervals: As we have derive the Gaussian quadrature formula over the interval $[-1,1]$ but we can easily change intervals from $[-1,1]$ to $[a,b]$ with

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the transformation $x = \frac{1}{2}(b-a)t + \frac{(a+b)}{2}$.

Then, a Gaussian quadrature rule of the form

$$\int_{-1}^{1} f(t)\,dt \approx \sum_{i=0}^{n} A_i f(t_i)$$

can be used over the interval $[a,b]$ as

$$\int_a^b f(x)\,dx = \frac{1}{2}(b-a)\int_{-1}^{1} f\left[\frac{1}{2}(b-a)t + \frac{1}{2}(b+a)\right] dt \quad \text{—— (3)}$$

**Que** Use Gaussian quadrature formula, to approximate the integral $\int_0^1 e^{-x^2}dx$ with three Gaussian nodes.

**Sol** Since $a=0$ and $b=1$, we have

$$\int_0^1 f(x)\,dx = \frac{1}{2}\int_{-1}^{1} f\left(\frac{1}{2}t + \frac{1}{2}\right) dt \quad \text{by (3)}$$

$$\approx \frac{1}{2}\left[\frac{5}{9} f\left(\frac{1}{2} - \frac{1}{2}\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f\left(\frac{1}{2}\right) + \frac{5}{9} f\left(\frac{1}{2} + \frac{1}{2}\sqrt{\frac{3}{5}}\right)\right]$$

(by Gaussian quadrature formula ②)

Here $f(x) = e^{-x^2}$

$$\therefore \int_0^1 e^{-x^2}dx \approx \frac{5}{18} e^{-0.112701665^2} + \frac{4}{9} e^{-0.5^2} + \frac{5}{18} e^{-0.887298335^2}$$

$$\approx 0.746814584$$

Ans

**Note:** Gaussian quadrature formula with two Gaussian nodes

$$\int_{-1}^{1} f(x)\,dx = f\left(-\sqrt{\frac{1}{3}}\right) + f\left(\sqrt{\frac{1}{3}}\right)$$

(To prove this take $c_1 = 0$ & so $q(x) = c_0 + c_2x^2$)

Similarly we can find Gaussian quadrature formula with only one node is $\int_{-1}^{1} f(x)\,dx = 2f(0)$ (To prove this $q(x) = c_0 + c_1x$)

**Note:** Do More Nodes (4 and 5) from your text book.