Chapter 6: Numerical Integration

In this chapter, we find the approximate value of the numerical integration. The basic method involved in approximating $\int_a^b f(x)dx$ is called **numerical quadrature**. It uses a sum $\sum_{i=0}^n a_i f(x_i)$ to approximate $\int_a^b f(x)dx$ $i.e.$ $\int_a^b f(x)dx \approx \sum_{i=0}^n a_i f(x_i)$.

How to get formula for the solving integration (approximately):

Divide the interval $[a,b]$ in to a set of $n+1$ distinct nodes $\{x_0, x_1, x_2, \dots, x_n\}$. Now, we approximate $f(x)$ by Lagrange's interpolating polynomials which is used to approximate $f(x)$. Thus, we can write $f(x) = P_n(x) + e_n(x)$

$$= \sum_{i=0}^n L_i(x) f(x_i) + \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^n (x - x_i),$$

where $\xi = \xi(x) \in [a,b]$ and $L_i(x)$

$$= \prod_{\substack{i=0 \\ i \neq k}}^n \frac{(x - x_i)}{(x_k - x_i)}.$$

Therefore

$$\begin{aligned} \int_a^b f(x)dx &= \int_a^b P_n(x)dx + \int_a^b e_n(x)dx \\ &= \int_a^b \sum_{i=0}^n f(x_i) L_i(x)\, dx + \int_a^b \prod_{i=0}^n (x - x_i) \frac{f^{(n+1)}(\xi(x))}{(n+1)!}\, dx \end{aligned}$$

$$= \sum_{i=0}^n a_i f(x_i) + E(f), \qquad \text{(say)}$$

where $a_i = \int_a^b L_i(x)dx$, for each $i = 0, 1, \dots, n$.

The quadrature formula is, therefore,

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

with error given by

$$E(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^n (x - x_i) f^{(n+1)}(\xi(x))\, dx.$$

Notes:

1. We can also use Newton interpolation to approximate the function $f(x)$.
2. The quadrature formula is called Newton-Cotes formula if all points are equally spaced.

Before discussing general quadrature formulas, let us derive formulas by using one and two degree interpolating polynomials with equally spaced nodes. This gives :

1. **Trapezoidal Rule** (derive from linear interpolating polynomial)
2. **Simpson's Rule** (derive from quadratic interpolating polynomial).

The Trapezoidal Rule

To derive the Trapezoidal rule for approximating $\int_a^b f(x)\,dx$, let $x_0 = a, x_1 = b, h = b - a$ and use the linear Lagrange polynomial:

$$P_1(x) = \frac{(x-x_1)}{(x_0-x_1)} f(x_0) + \frac{(x-x_0)}{(x_1-x_0)} f(x_1) = \sum_{i=0}^{1} L_i(x)\, f(x_i).$$

Then

$$f(x) = \sum_{i=0}^{1} L_i(x)\, f(x_i) + \frac{f''(\xi)}{2!}(x-x_0)(x-x_1), \quad \xi \in (x_0, x_1) = (a, b)$$

$$\Rightarrow \int_a^b f(x)dx = \int_{a=x_0}^{b=x_1} \left(\frac{(x-x_1)}{(x_0-x_1)} f(x_0) + \frac{(x-x_0)}{(x_1-x_0)} f(x_1) \right) dx$$

$$+ \int_{a=x_0}^{b=x_1} \frac{f''(\xi)}{2!}(x-x_0)(x-x_1)dx \coloneqq \sum_{i=0}^{1} a_i f(x_i) + E(f) \quad (say).$$

Where $a_0 = \int_{a=x_0}^{b=x_1} \left(\frac{(x-x_1)}{(x_0-x_1)} f(x_0) \right) dx$ and $a_1 = \int_{a=x_0}^{b=x_1} \left(\frac{(x-x_0)}{(x_1-x_0)} f(x_1) \right) dx$

$$= \frac{f(x_0)}{(x_0-x_1)} \left(\frac{(x-x_1)^2}{2} \right)_{x_0}^{x_1} \qquad = \frac{f(x_1)}{(x_1-x_0)} \left(\frac{(x-x_0)^2}{2} \right)_{x_0}^{x_1}$$

$$= \frac{x_1-x_0}{2} f(x_0) = \frac{h}{2} f(x_0) \qquad = \frac{x_1-x_0}{2} f(x_1) = \frac{h}{2} f(x_1).$$

Thus, approximate formula for $\int_a^b f(x)dx \approx \frac{h}{2}[f(x_0) + f(x_1)] = \frac{h}{2}[f(a) + f(b)]$.

The error term is given by

$$E(f) = \int_{x_0}^{x_1} \frac{f''(\xi)}{2!}(x-x_0)(x-x_1)dx$$

$$= \frac{1}{2!} \int_{x_0}^{x_1} f''(\xi)(x-x_0)(x-x_1)dx.$$

Since, $(x-x_0)(x-x_1)$ does not change its sign in $[x_0, x_1]$, therefore by using Weighted Mean Value Theorem*, there exists $c \in (x_0, x_1)$ such that

$$E(f) = \frac{f''(c)}{2!} \int_{x_0}^{x_1} (x-x_0)(x-x_1)dx$$

$$= \frac{f''(c)}{2} \frac{(x_0-x_1)^3}{6} = \frac{-h^3}{12} f''(c).$$

Thus the integration formula is

$$\boldsymbol{\int_a^b f(x)dx = \frac{h}{2}\big(f(a) + f(b)\big) - \frac{h^3}{12} f''(c).}$$

This is called Trapezoidal rule because $\int_a^b f(x)dx$ is approximated by the area of trapezium i.e. shaded portion in the following fig.1.

***Weighted Mean Value Theorem:** Let $f(x)$ is continuous on $[a, b]$ and $g(x)$ is integrable on $[a, b]$ and does not change sign in $[a, b]$, then $\int_a^b f(x)g(x)dx = f(c) \int_a^b g(x)dx$, for some $c \in (a, b)$.

(take $f = f''$, $g(x) = (x-x_0)(x-x_1)$ in above derivation for use).

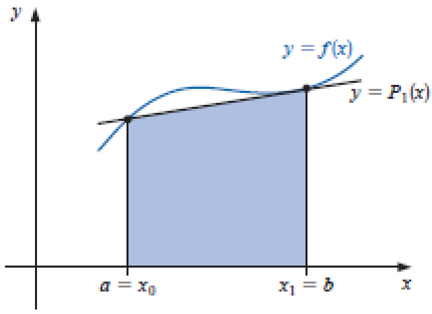


Fig.1

The error term for the Trapezoidal rule involves f'', so the rule gives the exact result when applied to any function whose second derivative is identically zero, that is, any polynomial of degree one or less.

Simpson's Rule

To derive Simpson's rule for approximating $\int_a^b f(x)dx$, we use second degree Lagrange's interpolating polynomials $P_2(x)$ with equally spaced nodes $x_0 = a,\ x_2 = b$ and $x_1 = a + h = \frac{a+b}{2}$, where $h = \frac{b-a}{2}$,

$$P_2(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)$$
$$= \sum_{i=0}^{2} L_i(x) f(x_i).$$

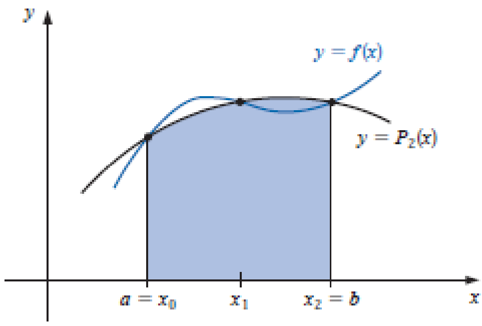


Fig. 2

Therefore, $f(x) = \sum_{i=0}^{2} L_i(x) f(x_i) + \frac{f'''(\xi)}{3!}(x - x_0)(x - x_1)(x - x_2), \quad \xi \in (x_0, x_2)$

$\Rightarrow$

$$\int_a^b f(x)dx = \int_{a=x_0}^{b=x_2} \left(\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right) dx$$

$$+ \int_{a=x_0}^{b=x_2} \frac{f'''(\xi)}{3!} (x - x_0)(x - x_1)(x - x_2) dx \coloneqq \sum_{i=0}^{2} a_i f(x_i) + E(f) \quad (say).$$

Where $a_0 = \int_{a=x_0}^{b=x_2} \left(\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) \right) dx$, $a_1 = \int_{a=x_0}^{b=x_2} \left(\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \right) dx$,

$$a_2 = \int_{a=x_0}^{b=x_2} \left(\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right) dx$$

By substituting $x = x_0 + ht, dx = h\,dt$ and change limits from 0 to 2, we obtain

$$a_0 = \frac{h}{3}, \quad a_1 = \frac{4\,h}{3}, \quad a_2 = \frac{h}{3}.$$

Thus, approximate formula for $\int_a^b f(x)dx \approx \frac{h}{3}[f(x_0) + 4\,f(x_1) + f(x_2)]$

$$= \frac{h}{3}\left[f(a) + 4\,f\left(\frac{a+b}{2}\right) + f(b)\right].$$

The error term is given by $E(f) = \int_{x_0}^{x_2} \frac{f'''(\xi)}{3!}(x - x_0)(x - x_1)(x - x_2)dx$

$$= \frac{1}{3!}\int_{x_0}^{x_2} f'''(\xi)(x - x_0)(x - x_1)(x - x_2)dx.$$

Since, $(x - x_0)(x - x_1)(x - x_2)$ changes its sign in $[x_0, x_2]$, therefore we can not apply Weighted Mean Value Theorem*. Moreover, $\int_{x_0}^{x_2} (x - x_0)(x - x_1)(x - x_2)dx = 0$.

Here we can add one more interpolation point without affecting the area of integration, leaving the error unaffected. Therefore, we simply repeat any one of the nodes $a = x_0, x_1, x_2 = b$ in the interval $[a, b]$. Suppose we repeat point x_1, then the interpolating points will be $a = x_0, x_1 = \frac{a+b}{2}, x_1 = \frac{a+b}{2}, x_2 = b$.

Thus error term becomes

$$E(f) = \frac{1}{4!}\int_{x_0}^{x_2} f^{iv}(\xi)(x - x_0)(x - x_1)^2(x - x_2)dx.$$

Since $(x - x_0)(x - x_1)^2(x - x_2)$ does not change its sign in $[x_0, x_2]$, therefore by using Weighted Mean Value Theorem*, there exists $c \in (x_0, x_2)$ such that

$$E(f) = \frac{f^{iv}(c)}{4!}\int_{x_0}^{x_1} (x - x_0)(x - x_1)^2(x - x_2)dx$$

$$= -\frac{f^{iv}(c)}{4!}\frac{(x_2-x_0)^5}{120} = -\frac{(2\,h)^5}{2880}f^{iv}(c) = -\frac{h^5}{90}f^{iv}(c).$$

Thus the integration formula is

$$\boldsymbol{\int_a^b f(x)dx = \frac{h}{3}[f(a) + 4\,f(\tfrac{a+b}{2}) + f(b)] - \frac{h^5}{90}f^{iv}(c).}$$

This is called Simpson rule. Because of $\frac{1}{3}$ factor, it is also referred to as Simpson's 1/3 rule.

The error term in Simpson's rule involves the fourth derivative of f, so it gives exact results when applied to any polynomial of degree three or less.

Example 1 Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)\,dx$ when $f(x)$ is

(a) x^2 **(b)** x^4 **(c)** $(x+1)^{-1}$

Find the absolute error and maximum bound for the errors.

Solution

(a) For $f(x) = x^2$, exact value = $\int_0^2 x^2dx = \frac{8}{3}$.

By trap. Rule, given values are $a = 0,\ b = 2,\ h = b - a = 2 - 0 = 2$

Trapezoid: $\int_0^2 f(x)\,dx \approx f(0) + f(2)$

For $f(x) = x^2$, $\int_0^2 x^2dx = \frac{2}{2}(0^2 + 2^2) = 4$.

Absolute error is $\left|4 - \frac{8}{3}\right| = \frac{4}{3}$.

and maximum error bound by Trap. Rule is

$$E(f) \le \frac{h^3}{12} \max_{0\le c\le 2} |f''(c)| = \frac{8}{12} * 2 = \frac{4}{3}.$$

By Simpson's1/3 Rule, given values are $a = 0,\ b = 2,\ h = \frac{b-a}{2} = 1.$

$$\text{Simpson's:} \quad \int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

For $f(x) = x^2$, $\int_0^2 x^2 dx = \frac{1}{3}(0^2 + 4 * 1^2 + 2^2) = \frac{8}{3}$, which is same as the exact value.

The approximation from Simpson's rule is exact because its truncation error involves $f^{(4)}$, which is identically 0 when $f(x) = x^2$.

(b) For $f(x) = x^4$, exact value $= \int_0^2 x^4 dx = \frac{32}{5}$.
By trap. Rule, given values are $a = 0,\ b = 2,\ h = b - a = 2 - 0 = 2$

$$\text{Trapezoid:} \quad \int_0^2 f(x)\,dx \approx f(0) + f(2)$$

For $f(x) = x^4$, $\int_0^2 x^4 dx = \frac{2}{2}(0^4 + 2^4) = 16.$

Absolute error is $\left|16 - \frac{32}{5}\right| = \frac{48}{5}$

and maximum error bound by Trap. Rule is

$$E(f) \le \frac{h^3}{12} \max_{0\le c\le 2} |f''(c)| = \frac{8}{12} * \max_{0\le c\le 2} 12\,c^2 = 32.$$

By Simpson's1/3 Rule, given values are $a = 0,\ b = 2,\ h = \frac{b-a}{2} = 1.$

$$\text{Simpson's:} \quad \int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

For $f(x) = x^4$, $\int_0^2 x^4 dx = \frac{1}{3}(0^4 + 4 * 1^4 + 2^4) = \frac{20}{3}$.

Absolute error is $\left|\frac{20}{3} - \frac{32}{5}\right| = \frac{4}{15}$

and maximum error bound by simpson's 1/3 Rule is

$$E(f) \le \frac{h^5}{90} \max_{0\le c\le 2} |f^{iv}(c)| = \frac{1^5}{90} * 24 = \frac{4}{15}.$$

(c) For $f(x) = \frac{1}{1+x}$, exact value $= \int_0^2 \frac{1}{1+x} dx = \ln(3) = 1.0986.$
By trap. Rule, given values are $a = 0,\ b = 2,\ h = b - a = 2 - 0 = 2$

$$\text{Trapezoid:} \quad \int_0^2 f(x)\,dx \approx f(0) + f(2)$$

For $\quad f(x) = \frac{1}{1+x}$, $\quad \int_0^2 \frac{1}{1+x} dx = \frac{2}{2}\left(\frac{1}{1+0} + \frac{1}{1+2}\right) = \frac{4}{3}$.

Absolute error is $\quad \left|\frac{4}{3} - \ln(3)\right| = \mathbf{0.2347.}$

and maximum error bound by Trap. Rule is

$$E(f) \leq \frac{h^3}{12} \max_{0\leq c\leq 2} |f''(c)| = \frac{8}{12} * \max_{0\leq c\leq 2} \frac{2}{(1+c)^3} = \frac{4}{3}.$$

By Simpson's1/3 Rule, given values are $a = 0,\ b = 2,\ h = \frac{b-a}{2} = 1$.

$$\text{Simpson's:} \quad \int_0^2 f(x)\,dx \approx \frac{1}{3}[f(0) + 4f(1) + f(2)].$$

For $\quad f(x) = \frac{1}{1+x}$, $\quad \int_0^2 \frac{1}{1+x} dx = \frac{1}{3}\left(\frac{1}{1+0} + 4 * \frac{1}{1+1} + \frac{1}{1+2}\right) = \frac{10}{9}$.

Absolute error is $\quad \left|\frac{10}{9} - \ln(3)\right| = \mathbf{0.0125}$

and maximum error bound by simpson's1/3 Rule is

$$E(f) \leq \frac{h^5}{90} \max_{0\leq c\leq 2} |f^{iv}(c)| = \frac{1^5}{90} * \max_{0\leq c\leq 2} \frac{24}{(1+c)^5} = \frac{4}{15}.$$

Measuring Precision

The standard derivation of quadrature error formulas is based on determining the class of polynomials for which these formulas produce exact results. The next definition is used to facilitate the discussion of this derivation.

Definition

The **degree of accuracy**, or **precision**, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \ldots, n$. ■

Note:

1. The degree of precision of a quadrature formula (general) is n if and only if the error is zero for all polynomials of degree $k = 0, 1, \ldots, n$, but is not zero for some polynomial of degree $n + 1$.
2. By definition of degree of accuracy, we can easily see that the trapezoidal and simpson's rules have degree of precision one and three respectively.
3. Note that when n is an even integer, the degree of precision is $n + 1$, although the interpolation polynomial is of degree at most n. When n is odd, the degree of precision is only n.
4. It is observed that higher degree of precision gives better accuracy. So, Simpson's 1/3 rule yields more accurate estimates than the Trapezoidal rule.

Example 2:

The quadrature formula $\int_0^2 f(x)\,dx = c_0 f(0) + c_1 f(1) + c_2 f(2)$ is exact for all polynomials of degree less than or equal to 2. Determine c_0, c_1, and c_2.

Solution The given quadrature formula is exact for all polynomials (monomials) degree less than or equal to 2. Therefore, we have

$$f(x) = 1: \qquad \int_0^2 1\, dx = 2 = c_0 + c_1 + c_2$$

$$f(x) = x: \qquad \int_0^2 x\, dx = 2 = c_1 + 2\, c_2$$

$$f(x) = x^2: \qquad \int_0^2 x^2\, dx = \frac{8}{3} = c_1 + 4\, c_2.$$

By solving these linear equations, we get $\boldsymbol{c_0 = \frac{1}{3}}$, $\boldsymbol{c_1 = \frac{4}{3}}$, $\boldsymbol{c_2 = \frac{1}{3}}$.

Example 3:

Find the constants c_0, c_1, and x_1 so that the quadrature formula

$$\int_0^1 f(x)\, dx = c_0 f(0) + c_1 f(x_1)$$

has the highest possible degree of precision.

Solution We make the given formula exact for all polynomials (monomials) degree less than or equal to 2 to get three equations in three unknowns.

$$f(x) = 1: \qquad \int_0^1 1\, dx = 1 = c_0 + c_1$$

$$f(x) = x: \qquad \int_0^1 x\, dx = \frac{1}{2} = c_1 x_1$$

$$f(x) = x^2: \qquad \int_0^1 x^2\, dx = \frac{1}{3} = c_1 x_1^2.$$

By solving these non-linear equations, we get $\boldsymbol{c_0 = \frac{1}{4}}$, $\boldsymbol{c_1 = \frac{3}{4}}$, $\boldsymbol{x_1 = \frac{2}{3}}$.

Composite Numerical Integration:

The Newton cotes formulas are generally unsuitable for use over large integration intervals. In that case, high-degree formulas would be required, and the values of the coefficients in these formulas are difficult to obtain. Moreover, order of the derivative and step size (h) between the nodes involved in error term also increase. Therefore, we can use composite numerical integration.

In this section, we discuss a piecewise approach to numerical integration that uses the low-order Newton-Cotes formulas.

Composite Trapezoidal Rule: We divide the interval $[a, b]$ into n subintervals with step size $h = \frac{b-a}{n}$, and taking nodal points $a = x_0 < x_1 < \cdots x_n = b$, where $x_i = x_0 + ih, i = 1,2, \ldots n$.

Let us take $\int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx.$

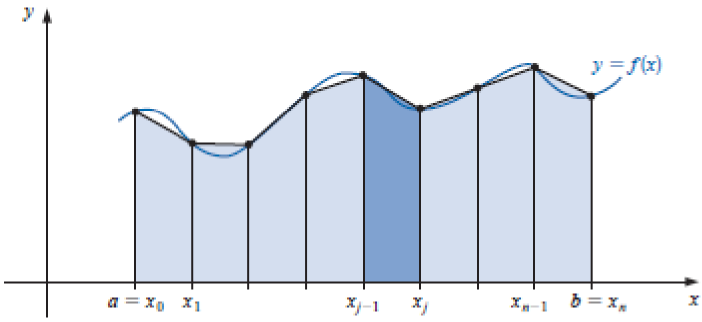
Now use trapezoidal rule for each of the integrals on the right side, we obtain

$$\int_a^b f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi_1) + \frac{h}{2}[f(x_1) + f(x_2)] - \frac{h^3}{12} f''(\xi_2) + \cdots$$

$$+ \frac{h}{2}[f(x_{n-1}) + f(x_n)] - \frac{h^3}{12} f''(\xi_n)$$

$$= \frac{h}{2}\left[f(x_0) + f(x_n) + 2\sum_{i=1}^{n-1} f(x_i)\right] - \frac{h^3}{12}\sum_{i=1}^{n} f''(\xi_i),$$

where $x_{i-1} \le \xi_i \le x_i, i = 1, 2, \ldots, n$.



Error term involved in composite trapezoidal rule is given by

$$E(f) = -\frac{h^3}{12}\sum_{i=1}^{n} f''(\xi_i).$$

If $f \in C^2[a,b]$, the Extreme Value Theorem** implies that f'' assumes its maximum and minimum value in $[a,b]$.

Since $\min_{x\in[a,b]} f''(x) \le f''(\xi_i) \le \max_{x\in[a,b]} f''(x)$, then we have

$$\sum_{i=1}^{n} \min_{x\in[a,b]} f''(x) \le \sum_{i=1}^{n} f''(\xi_i) \le \sum_{i=1}^{n} \max_{x\in[a,b]} f''(x)$$

$$\Rightarrow\ n \min_{x\in[a,b]} f''(x) \le \sum_{i=1}^{n} f''(\xi_i) \le n \max_{x\in[a,b]} f''(x)$$

$$\Rightarrow\ \min_{x\in[a,b]} f''(x) \le \frac{1}{n}\sum_{i=1}^{n} f''(\xi_i) \le \max_{x\in[a,b]} f''(x).$$

By Intermediate Value Theorem*** there exists $c \in (a,b) = (x_0, x_n)$ such that

$$f''(c) = \frac{1}{n}\sum_{i=1}^{n} f''(\xi_i).$$

Therefore $E(f) = -\frac{h^3}{12} n f''(c) = -\frac{h^2}{12}(b-a)f''(c)$, as $h = \frac{b-a}{n}$.

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

with error $E(f) = -\frac{\boldsymbol{h^2}}{\boldsymbol{12}}(\boldsymbol{b}-\boldsymbol{a})\boldsymbol{f''}(\boldsymbol{c}),\quad \boldsymbol{c} \in (\boldsymbol{a},\boldsymbol{b})$.

****Extreme Value Theorem:** It states that if a real valued function f is continuous on the closed interval $[a,b]$, then f must attain a minimum and a maximum, each at least once i.e. there exist numbers c and d in $[a,b]$ such that:

$$f(c) \le f(x) \le f(d), \qquad \text{for all } x \in [a,b].$$

(take $f = f''$, $f''(c) = \min_{x\in[a,b]} f''(x)$, $f''(d) = \max_{x\in[a,b]} f''(x)$ and for any $\xi_i \in [a,b]$ $\min_{x\in[a,b]} f''(x) \le f''(\xi_i) \le \max_{x\in[a,b]} f''(x)$ in above derivation for use).

*****Intermediate Value Theorem:** It states that if a real valued function f is continuous on the closed interval $[a,b]$, then it takes on any given value between $f(a)$ and $f(b)$ at some point within the interval i.e. if u is a number between $f(a)$ and $f(b)$, then there is $c \in [a,b]$ such that $f(c) = u$.

(take $f = f''$, $u = \frac{1}{n}\sum_{i=1}^{n} f''(\xi_i)$, in above derivation for use).

Composite Simpson'1/3 Rule: For simpson's rule, we divide the interval $[a, b]$ into two (even) equal subintervals and get three (odd) nodal points. Therefore, we choose an even integer $N(=2n)$. Subdivide the interval $[a, b]$ into $N(=2n)$ subintervals, with step size $h=\frac{b-a}{2n}$, and taking nodal points $a=x_0<x_2<\cdots x_{2n}=b$, where $x_i=x_0+ih, i=1,2, \ldots 2n$.

Let us take $\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \cdots + \int_{x_{2n-2}}^{x_{2n}} f(x)dx$.

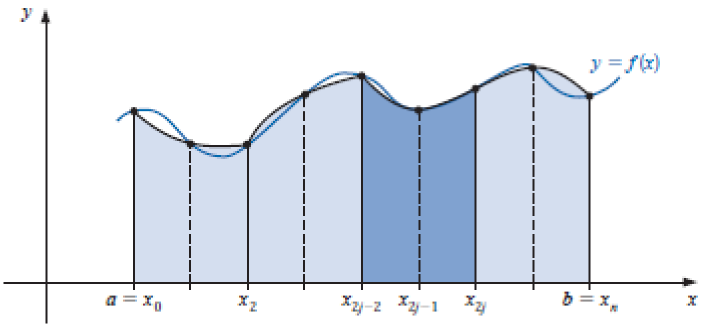
Now use simpson's rule for each of the integrals on the right side, we obtain

$$\int_a^b f(x)dx = \frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)] - \frac{h^5}{90} f^{iv}(\xi_1) + \frac{h}{3}[f(x_2)+4f(x_3)+f(x_4)]$$

$$-\frac{h^5}{90} f^{iv}(\xi_2) + \cdots + \frac{h}{3}[f(x_{2n-2})+4f(x_{2n-1})+f(x_{2n})] - \frac{h^5}{90} f^{iv}(\xi_n)$$

$$= \frac{h}{3}\left[f(x_0)+f(x_{2n}) + 2\sum_{i=1}^{n-1} f(x_{2i}) + 4\sum_{i=1}^{n} f(x_{2i-1})\right] - \frac{h^5}{90}\sum_{i=1}^{n} f^{iv}(\xi_i),$$

where $x_{2i-2} \le \xi_i \le x_{2i}, i=1,2,\ldots,n$.



Error term involved in composite Simpson's rule is given by

$$E(f) = -\frac{h^5}{90}\sum_{i=1}^{n} f^{iv}(\xi_i).$$

If $f \in C^4[a,b]$, the Extreme Value Theorem implies that f^{iv} assumes its maximum and minimum value in $[a, b]$.

Since $\min_{x\in[a,b]} f^{iv}(x) \le f^{iv}(\xi_i) \le \max_{x\in[a,b]} f^{iv}(x)$, then we have

$$\sum_{i=1}^{n} \min_{x\in[a,b]} f^{iv}(x) \le \sum_{i=1}^{n} f^{iv}(\xi_i) \le \sum_{i=1}^{n} \max_{x\in[a,b]} f^{iv}(x)$$

$$\Rightarrow \; n \min_{x\in[a,b]} f^{iv}(x) \le \sum_{i=1}^{n} f^{iv}(\xi_i) \le n \max_{x\in[a,b]} f^{iv}(x)$$

$$\Rightarrow \; \min_{x\in[a,b]} f^{iv}(x) \le \frac{1}{n}\sum_{i=1}^{n} f^{iv}(\xi_i) \le \max_{x\in[a,b]} f^{iv}(x).$$

By Intermediate Value Theorem there exists $c \in (a,b)=(x_0,x_n)$ such that

$$f^{iv}(c) = \frac{1}{n}\sum_{i=1}^{n} f^{iv}(\xi_i).$$

Therefore $E(f) = -\frac{h^5}{90} n f^{iv}(c) = -\frac{h^4}{180}(b-a) f^{iv}(c)$, as $h=\frac{b-a}{2n}$.

Thus composite simpson's 1/3 formula is

$$\frac{\boldsymbol{h}}{\mathbf{3}}\left[\mathbf{f}(\mathbf{x}_0) + \mathbf{f}(\mathbf{x}_{2n}) + \mathbf{2}\sum_{i=1}^{n-1} \mathbf{f}(\mathbf{x}_{2i}) + \mathbf{4}\sum_{i=1}^{n} \mathbf{f}(\mathbf{x}_{2i-1})\right]$$

with error $E(f) = -\frac{\boldsymbol{h}^4}{\mathbf{180}}(\boldsymbol{b}-\boldsymbol{a})\boldsymbol{f}^{iv}(\boldsymbol{c}), \quad \boldsymbol{c} \in (\boldsymbol{a}, \boldsymbol{b})$.

Notes:

1. In trapezoidal rule, n can by any positive integer whereas, in simpson's rule n must be an even positive integer i.e. number of nodal points must be odd.
2. The accuracy can be improved by increasing n.

Example 4: Use composite trapezoidal rule and composite simpson's 1/3 rule integrals with $n = 6$ to approximate the integral $\int_0^2 \sin 3x \ dx$.

Solution: Trap. Rule: Let $f(x) = \sin 3x$. By taking $a = 0, b = 2, n = 6$, with $h = \frac{b-a}{6} = \frac{1}{3}$, the nodal points

$x_0 = 0, x_1 = \frac{1}{3}, x_2 = \frac{2}{3}, x_3 = 1, x_4 = \frac{4}{3}, x_5 = \frac{5}{3}, x_6 = \frac{6}{3} = 2$, we obtain

$$\int_0^2 \sin 3x \ dx = \frac{\frac{1}{3}}{2}\left[f(0) + f(2) + 2\left(f\left(\frac{1}{3}\right) + f\left(\frac{2}{3}\right) + f(1) + f\left(\frac{4}{3}\right) + f\left(\frac{5}{3}\right)\right)\right]$$
$$= \mathbf{0.01215}.$$

Simpson's Rule: Let $f(x) = \sin 3x$. By taking $a = 0, b = 2, N = 6$, with $h = \frac{b-a}{6} = \frac{1}{3}$, the nodal points

$x_0 = 0, x_1 = \frac{1}{3}, x_2 = \frac{2}{3}, x_3 = 1, x_4 = \frac{4}{3}, x_5 = \frac{5}{3}, x_6 = \frac{6}{3} = 2$, we obtain

$$\int_0^2 \sin 3x \ dx = \frac{\frac{1}{3}}{3}\left[f(0) + f(2) + 2\left(f\left(\frac{2}{3}\right) + f\left(\frac{4}{3}\right)\right) + 4\left(f\left(\frac{1}{3}\right) + f(1) + f\left(\frac{5}{3}\right)\right)\right]$$
$$= \mathbf{0.01336}.$$

Exact value $\int_0^2 \sin 3x \ dx = 0.01328$.

Example 5:

Determine the values of n and h required to approximate

$$\int_0^2 \frac{1}{x+4}\, dx$$

to within 10^{-3} and compute the approximation. Use

a. Composite Trapezoidal rule.

b. Composite Simpson's rule.

Solution: Let $f(x) = \frac{1}{x+4} \Rightarrow f''(x) = \frac{2}{(x+4)^3}$ and $f^{iv}(x) = \frac{24}{(x+4)^5}$

$\max_{x\in[0,2]} |f''(x)| = \frac{2}{4^3} = \frac{1}{32}$, $\max_{x\in[0,2]} |f^{iv}(x)| = \frac{24}{4^5} = \frac{3}{128}$.

(a) Error in composite trapezoidal rule is given by

$$E(f) = -\frac{h^2}{12}(b-a)f''(c), \quad c \in (0,2).$$

Given that

$$\max_{c\in(0,2)} E(f) \le 10^{-3}$$
$$\max_{c\in(0,2)} \frac{h^2}{12}(2-0)|f''(c)| \le 10^{-3}$$
$$\frac{h^2}{6}\frac{1}{32} \le 10^{-3}$$

$$\boldsymbol{h \le 0.192} \Rightarrow n = \frac{b-a}{h} \ge \frac{2}{0.192} = 10.42 \Rightarrow \boldsymbol{n = 11}.$$

By taking $a = 0, b = 2, n = 11$, with $h = \frac{b-a}{11} = \frac{2}{11}$, the nodal points $x_0 = 0, x_1 = \frac{2}{11}, x_2 = \frac{4}{11}, x_3 = \frac{6}{11}, x_4 = \frac{8}{11}, x_5 = \frac{10}{11}, x_6 = \frac{12}{11}, x_7 = \frac{14}{11}, x_8 = \frac{16}{11}, x_9 = \frac{18}{11}, x_{10} = \frac{20}{11}, x_{11} = \frac{22}{11} = 2$, we obtain

$$\int_0^2 \frac{1}{x+4}\, dx = \frac{\frac{2}{11}}{2}\Bigg[f(0) + f(2) + 2\left(f\left(\frac{2}{11}\right) + f\left(\frac{4}{11}\right) + f\left(\frac{6}{11}\right) + f\left(\frac{8}{11}\right) + f\left(\frac{10}{11}\right) + f\left(\frac{12}{11}\right) + f\left(\frac{14}{11}\right) + f\left(\frac{16}{11}\right) + f\left(\frac{18}{11}\right) + f\left(\frac{20}{11}\right)\right)\Bigg]$$

$$= \mathbf{1.1011.}$$

(b) Error in composite simpson's rule is given by

$$E(f) = -\frac{h^4}{180}(b-a)f^{iv}(c), \quad c \in (0,2).$$

Given that

$$\max_{c\in(0,2)} E(f) \le 10^{-3}$$

$$\max_{c\in(0,2)} \frac{h^4}{180}(b-a)|f^{iv}(c)| \le 10^{-3}$$

$$\frac{h^4}{180}\frac{2*3}{128} \le 10^{-3}$$

$$\boldsymbol{h \le 1.3999} \Rightarrow N = \frac{b-a}{h} \ge \frac{2}{1.3999} = 1.4287,$$

$$\Rightarrow \boldsymbol{N = 2}.\ (\boldsymbol{even\ integer})$$

By taking $a = 0, b = 2, N = 2$, with $h = \frac{b-a}{2} = \frac{2}{2} = 1$, the nodal points $x_0 = 0, x_1 = 1, x_2 = 2$, we obtain

$$\int_0^2 \frac{1}{x+4}\, dx = \frac{1}{3}[f(0) + f(2) + 4f(1)]$$

$$= \mathbf{1.1111.}$$

Exact value $\int_0^2 \frac{1}{1+x}\, dx = \ln 3 = 1.0986$

Example 6: Determine the values of subintervals n and step-size h required to approximate $\int_0^2 \sin x\ dx$ to within 10^{-2} and hence compute the approximation using composite Simpson's rule.

Solution: Let $f(x) = \sin x \Rightarrow f^{iv}(x) = \sin x$

$\max_{x\in[0,2]} |f^{iv}(x)| = 1.$

Error in composite simpson's rule is given by

$$E(f) = -\frac{h^4}{180}(b-a)f^{iv}(c), \quad c \in (0,2).$$

Given that

$$\max_{c\in(0,2)} E(f) \le 10^{-2}$$

$$\max_{c\in(0,2)} \frac{h^4}{180}(b-a)|f^{iv}(c)| \le 10^{-2}$$

$$\frac{h^4}{180} 2 * 1 \leq 10^{-2}$$

$$\boldsymbol{h \leq 0.9740} \Rightarrow N = \frac{b-a}{h} \geq \frac{2}{0.9740} = 2.0534$$

$$\Rightarrow \boldsymbol{N = 4}\ (\boldsymbol{next\ even\ integer}).$$

By taking $a = 0, b = 2, N = 4$, with $h = \frac{b-a}{4} = \frac{2}{4} = \frac{1}{2}$, the nodal points $x_0 = 0, x_1 = \frac{1}{2}, x_2 = 1, x_3 = \frac{3}{2}, x_4 = 2,$ we obtain

$$\int_0^2 \sin x\ dx = \frac{1}{6}\left[f(0) + f(2) + 2f(1) + 4\left(f\left(\frac{1}{2}\right) + f\left(\frac{3}{2}\right)\right)\right]$$

$$= \mathbf{1.4166.}$$

Exact value $\int_0^2 \sin x\ dx = 1.4161.$

Remark: The Newton-Cotes formulas were derived by integrating interpolating polynomials. The error term in the interpolating polynomial of degree n involves the $(n+1)th$ derivative of the function being approximated, so a Newton-Cotes formula is exact when approximating the integral of any polynomial of degree less than or equal to n.

Limitations of Newton-cotes formulas:

All the Newton-Cotes formulas use values of the function at equally-spaced points. This restriction is convenient when the formulas are combined to form the composite rules but it can significantly decrease the accuracy of the approximation.

Gaussian Quadrature:

Newton Cotes formulas pick equally spaced points in the interval of integration, Gaussian quadrature chooses the best points for evaluation rather than equally spaced, way. For this reason Gaussian quadrature is more accurate.

In the numerical integration method

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} \lambda_i f(x_i),$$

if both nodes x_i and multipliers λ_i are unknown then method is called Gaussian quadrature.

The coefficients $\lambda_1, \lambda_2, \ldots, \lambda_n$ in the approximation formula are arbitrary, and the nodes $x_1, x_2, \ldots, x_n$ are restricted only by the fact that they must lie in $[a, b]$. This gives us $2n$ unknowns to choose. We can obtain these unknowns by making the method exact for the class of polynomials of degree at most $2n - 1$ which gives $2n$ equations in these $2n$ unknowns. (as we have done in degree of precision section)

For this, we use **Legendre polynomials**, a collection $\{P_0(x), P_1(x), \ldots, P_n(x), \ldots\}$ with properties:

1. For each n, $P_n(x)$ is a monic polynomial of degree n.
2. $\int_{-1}^{1} P(x)P_n(x)dx = 0$, whenever $P(x)$ is a polynomial of degree less than n.
3.

The first few Legendre polynomials are

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = x^2 - \frac{1}{3},$$

$$P_3(x) = x^3 - \frac{3}{5}x, \quad \text{and} \quad P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}.$$

4. The roots of these polynomials are distinct, lie in the interval $(-1,1)$ have a symmetry with respect to the origin, and, most importantly, are the correct choice for determining the parameters that give us the nodes and coefficients for our quadrature method.

Gauss-Legendre Integration Methods:

The Gaussian quadrature formulas are derived for the interval $[-1,1]$ and any interval $[a,b]$ can be transformed to $[-1,1]$ by taking the transformation $x = ct + d$, which gives $a = -c + d$ and $b = c + d \Rightarrow x = \frac{b-a}{2}t + \frac{b+a}{2}$.

One-point formula: For $n = 1$, the formula is given by $\int_{-1}^{1} f(x)dx = \lambda_0 f(x_0)$.

The method has two unknowns λ_0 and x_0. Make the method exact for $f(x) = 1, x$, we obtain

For $f(x) = 1$, we get $\int_{-1}^{1} 1\, dx = \lambda_0 \,.1 \quad \Rightarrow 2 = \lambda_0$

For $f(x) = x$, we get $\int_{-1}^{1} x\, dx = \lambda_0 \,.x_0 \quad \Rightarrow 0 = \lambda_0 x_0 \quad \Rightarrow 2\,x_0 = 0 \quad \Rightarrow x_0 = 0.$

Therefore one point formula is given by $\boldsymbol{\int_{-1}^{1} f(x)dx = 2\,f(0).}$

Two-point formula: For $n = 2$, the formula is given by $\int_{-1}^{1} f(x)dx = \lambda_0 f(x_0) + \lambda_1 f(x_1)$.

The method has four unknowns $\lambda_0, \lambda_1, x_0$ and x_1. Make the method exact for $f(x) = 1, x, x^2, x^3$, we obtain

For $f(x) = 1$, we get $\int_{-1}^{1} 1\, dx = \lambda_0 \,.1 + \lambda_1 \,.1 \quad \Rightarrow 2 = \lambda_0 + \lambda_1 \quad (1)$

For $f(x) = x$, we get $\int_{-1}^{1} x\, dx = \lambda_0 \,.x_0 + \lambda_1 .x_1 \quad \Rightarrow 0 = \lambda_0 x_0 + \lambda_1 x_1 \quad (2)$

For $f(x) = x^2$, we get $\int_{-1}^{1} x^2\, dx = \lambda_0 \,.x_0^2 + \lambda_1 .x_1^2 \quad \Rightarrow \frac{2}{3} = \lambda_0 x_0^2 + \lambda_1 x_1^2 \quad (3)$

For $f(x) = x^3$, we get $\int_{-1}^{1} x^3\, dx = \lambda_0 \,.x_0^3 + \lambda_1 .x_1^3 \quad \Rightarrow 0 = \lambda_0 x_0^3 + \lambda_1 x_1^3. \quad (4)$

Eliminate λ_0 and x_0, form (2) and (4) equations, we get

$$\lambda_1 .x_1^3 - \lambda_1 .x_0^2\, x_1 = 0$$

$$\Rightarrow \quad \lambda_1 .x_1(x_1 - x_0)(x_1 + x_0) = 0.$$

Since $\lambda_0 \neq 0$ and $\lambda_1 \neq 0$, ($\because$ if $\lambda_0 = 0$ or $\lambda_1 = 0$, then formula reduces to one-point formula), $x_1 - x_0 \neq 0$ ($\because$ both nodes can't be same, otherwise again it will reduces to one-point formula) and $x_1 \neq 0$ ($\because$ if $x_1 = 0$, then from (2), $\lambda_0 x_0 = 0 \Rightarrow x_0 = 0 \Rightarrow x_1 = x_0$), then there is only one possibility

$$\text{i. e.} \quad x_1 = -x_0,$$

put it in (2), we get $\lambda_1 = \lambda_0$. From equation (1), we obtain $\lambda_1 = \lambda_0 = 1$. Putting these values in (3), we get $x_0 = \pm\frac{1}{\sqrt{3}}$ and $x_1 = \mp\frac{1}{\sqrt{3}}$.

Therefore, two-point formula is given by $\boldsymbol{\int_{-1}^{1} f(x)dx = f\left(\frac{1}{\sqrt{3}}\right) + f\left(\frac{-1}{\sqrt{3}}\right).}$

Three-point formula:

For $n = 3$, the formula is given by $\int_{-1}^{1} f(x)dx = \lambda_0 f(x_0) + \lambda_1 f(x_1) + \lambda_2 f(x_2)$.

The method has six unknowns, make it exact for $f(x) = 1, x, x^2, x^3, x^4, x^5$. After solving the 6 equations in 6 unknowns, we get $\boldsymbol{\int_{-1}^{1} f(x)dx = \frac{1}{9}\left[5f\left(\frac{\sqrt{3}}{\sqrt{5}}\right) + 8f(0) + 5f\left(\frac{-\sqrt{3}}{\sqrt{5}}\right)\right].}$

Example 7: Approximate the integral $\int_{0}^{\frac{\pi}{4}} (\cos x)^2 dx$ using Gauss-Legendre 1, 2 and 3 point formula. Also compare with the exact value.

Solution: Exact value of $\int_0^{\frac{\pi}{4}}(cos\ x)^2 dx = \mathbf{0.6427}.$

To apply Gauss-Legendre formulas, first we change the interval $[0, \frac{\pi}{4}]$ in to $[-1,1]$, by taking $x = \frac{\pi}{8}t + \frac{\pi}{8}, dx = \frac{\pi}{8}dt.$

We get $\int_0^{\frac{\pi}{4}}(cos\ x)^2 dx = \int_{-1}^{1} \cos^2 \frac{\pi}{8}(t+1) * \frac{\pi}{8}dt = \int_{-1}^{1} F(t)dt.$

By using 1 −point formula, $\int_{-1}^{1} \frac{\pi}{8}\cos^2 \frac{\pi}{8}(t+1)\, dt = 2\, F(0) = 2. \frac{\pi}{8} \cos^2\left(\frac{\pi}{4}\right) = \mathbf{0.3927}.$

By using 2 −point formula, $\int_{-1}^{1} \frac{\pi}{8}\cos^2 \frac{\pi}{8}(t+1)\, dt = F\left(\frac{1}{\sqrt{3}}\right) + F\left(\frac{-1}{\sqrt{3}}\right) = \mathbf{0.6423}.$

By using 3 −point formula, $\int_{-1}^{1} \frac{\pi}{8}\cos^2 \frac{\pi}{8}(t+1)\, dt = \frac{1}{9}\left[5F\left(\frac{\sqrt{3}}{\sqrt{5}}\right) + 8F(0) + 5F\left(\frac{-\sqrt{3}}{\sqrt{5}}\right)\right]$
$= \mathbf{0.6427}.$

For comparison, find absolute error of the values by these formulas and exact solution.

Example 8: Determine constants $a, b, c,$ and d that will produce a quadrature formula

$$\int_{-1}^{1} f(x)dx = af(-1) + bf(1) + cf'(-1) + df'(1)$$

that has degree of precision 3.

Solution The given formula has degree of precision 3. Therefore, it is exact for all polynomials (monomials) of degree less than or equal to 3.

$$f(x) = 1: \qquad \int_{-1}^{1} 1\, dx = 2 = a + b$$

$$f(x) = x: \qquad \int_{-1}^{1} x\, dx = 0 = -a + b + c + d$$

$$f(x) = x^2: \qquad \int_{-1}^{1} x^2\, dx = \frac{2}{3} = a + b - 2c + 2d$$

$$f(x) = x^3: \qquad \int_{-1}^{1} x^3\, dx = 0 = -a + b + 3c + 3d.$$

By solving these equations, we get $\boldsymbol{a = 1, b = 1, c = \frac{1}{3}, d = -\frac{1}{3}}.$