Numerical Integration:

Given a function f on $[a, b]$, the problem of numerical integration or numerical quadrature, is that of approximating the number

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

The problem arises when the integration cannot be carried out or the function $f(x)$ is known only at a finite number of points.

We approximate $I(f)$ by $I(P_n)$, where $P_n(x)$ is the polynomial of degree $\leq n$ which agrees with $f(x)$ at the points $x_0, x_1, \ldots x_n$. The approximation is usually written as a rule, as a weighted sum

$$I(P_n) = A_0 f(x_0) + A_1 f(x_1) + \cdots + A_n f(x_n)$$

of the function values $f(x_0), \ldots f(x_n)$. The weight could be calculated as $A_i = I(l_i)$, where l_i is the Lagrange polynomial correspond to x_i, i.e. $l_i(x_i) = 1$, $l_i(x_j) = 0$, $j \neq i$.

Assume that f is smooth on $[c, d] \supset [a, b]$.

Recall that $P_n(x)$ which agrees with $f(x)$ at $x_0, x_1, \ldots x_n$ is given by

$$P_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + \cdots + f[x_0, \ldots x_n] \prod_{j=0}^{n-1}(x - x_j)$$

Now suppose $P_{n+1}(x)$ agrees with $f(x)$ at the points $x_0, x_1, \ldots x_n, x$. Then

$$P_{n+1}(x) = P_n(x) + f[x_0, x_1, \ldots x_n, x] \prod_{j=0}^{n}(x - x_j)$$

Since $P_{n+1}(x) = f(x)$, for considered point x. (2)

we have

$$f(x) = P_n(x) + f[x_0, x_1, \dots x_n, x] \prod_{j=0}^{n} (x - x_j).$$

Define $\psi_n(x) = \prod_{j=0}^{n} (x - x_j)$. Then

$$f(x) = P_n(x) + f[x_0, x_1, \dots x_n, x] \, \psi_n(x).$$

We define $I(P_n)$ as an approximation to $I(f)$.

The Error $E(f) = I(f) - I(P_n)$ is given by

$$E(f) = \int_a^b f[x_0, x_1, \dots x_n, x] \, \psi_n(x) \, dx. \quad \text{—(1)}$$

If $f(x)$ is $(n+1)$ times continuously differentiable on $[a, b]$, then since $f[x_0, x_1, \dots x_n, x] = \dfrac{f^{(n+1)}(\xi(x))}{(n+1)!}$

for $\xi(x)$ lies between $x_0, x_1, \dots x_n, x$.

So
$$E(f) = \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \psi_n(x) \, dx$$

If $\psi_n(x)$ does not change sign on $[a, b]$, then

$$E(f) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \int_a^b \psi_n(x) \, dx. \quad \text{—(2)}$$

[Mean value theorem for integrals $\int_a^b g(x) h(x) = h(\xi) \int_a^b g(x) dx$, $g(x)$ does not change sign.]

In case if $\psi_n(x)$ is not of one sign on $[a, b]$, then we may obtain certain simplification when

$$\int_a^b \psi_n(x) \, dx = 0.$$

If $\int_a^b \psi_n(x)\,dx = 0$, then first note that (3)

$$f[x_0, x_1, \ldots x_{n+1}, x] = f[x_0, x_1, \ldots x_n, x_{n+1}] + f[x_0, \ldots x_{n+1}, x](x-x_{n+1})$$

and

$$E(f) = \int_a^b f[x_0, x_1, \ldots x_n, x]\,\psi_n(x)\,dx$$

$$= \int_a^b \underbrace{f[x_0, x_1, \ldots x_n, x_{n+1}]}_{\text{constant}}\,\psi_n(x)\,dx + \int_a^b f[x_0, \ldots x_{n+1}, x]\,\psi_{n+1}(x)\,dx$$

$$= f[x_0, x_1, \ldots x_{n+1}] \int_a^b \psi_n(x)\,dx + \int_a^b f[x_0, x_1, \ldots x_{n+1}, x]\,\psi_{n+1}(x)\,dx$$

$$= \int_a^b f[x_0, x_1, \ldots x_{n+1}, x]\,\psi_{n+1}(x)\,dx$$

If x_{n+1} is chosen in such a way that $\psi_{n+1}(x) = (x - x_{n+1})\,\psi_n(x)$ has one sign on (a, b)

then

$$E(f) = \int_a^b \frac{f^{(n+2)}(\xi(x))}{(n+2)!}\,\psi_{n+1}(x)\,dx$$

$$= \frac{f^{(n+2)}(\xi)}{(n+2)!} \int_a^b \psi_{n+1}(x)\,dx. \quad \text{— (3)}$$

Comparing (2) and (3), $(n+2)^{th}$ order derivative of f appears in (3) and we can expect higher order numerical integration from (3).

Specific Cases:

(1) $n=0$:

Then $f(x) = f[x_0] + f[x_0, x](x - x_0)$

Hence $I(P_0) = \int_a^b f[x_0]\,dx = (b-a) f(x_0)$.

If $x_0 = a$, then the approximation becomes

$$\boxed{I(f) \approx R = (b-a) f(a)}$$

This is called rectangular rule. Since in this case $\varphi_0(x) = x - x_0 = x - a$ is of one sign on $[a,b]$, the error E^R is given by

$$\boxed{E^R = f'(\eta) \int_a^b (x-a)\,dx = \frac{f'(\eta)(b-a)^2}{2}}$$

where $\eta \in (a,b)$.

If $x_0 = \frac{a+b}{2}$, then $\varphi_0(x)$ fails to be of one sign on (a,b). But then

$$\int_a^b \left(x - \frac{a+b}{2}\right) dx = 0,$$

while $\varphi_1(x) = (x-x_0)(x-x_0) = \left(x - \frac{a+b}{2}\right)^2$ is of one sign on (a,b). Hence in this case we obtain formula

$$\boxed{I(f) \approx M = (b-a) f\left(\frac{a+b}{2}\right)}$$

$\because \int_a^b f(x_0) = (b-a) f\left(\frac{a+b}{2}\right)$

and

$$\boxed{E^M = \frac{f''(\eta)(b-a)^3}{24}, \quad \eta \in (a,b)}$$

$\int_a^b (x-x_0)^2 = \frac{(b-a)^3}{12}$

$x_0 = \frac{a+b}{2}$.

This is called Mid point rule

Let $n=1$. Let

$$f(x) = P_1(x) + f[x_0, x_1, x]\,\psi_1(x),$$

where $P_1(x) = f[x_0] + f[x_0, x_1](x - x_0)$ and

$$\psi_1(x) = (x - x_0)(x - x_1).$$

To get $\psi_1(x)$ one sign on (a, b), we choose $x_0 = a$ and $x_1 = b$. Then by (2).

$$I(f) = \int_a^b \Big(f(a) + f[a,b](x-a) \Big)\,dx + \frac{f''(\eta)}{2} \int_a^b (x-a)(x-b)\,dx$$

or

$$\boxed{I(f) \approx T = \frac{1}{2}(b-a)\big(f(a) + f(b)\big).}$$

$$\boxed{E^T = -\frac{f''(\eta)}{12}(b-a)^3, \quad \eta \in (a,b).}$$

This is called trapezoidal rule.

Note that

$$\int_a^b \Big(f(a) + f[a,b](x-a) \Big)\,dx = f(a)(b-a) + f[a,b] \left.\frac{(x-a)^2}{2}\right|_a^b$$

$$= f(a)(b-a) + f[a,b]\frac{(b-a)^2}{2}$$

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

$$\int_a^b (x-a)(x-b)\,dx = \int_a^b \big(x^2 - (a+b)x + ab\big)\,dx = \left.\frac{x^3}{3} - (a+b)\frac{x^2}{2} + abx\right|_a^b$$

$$= \frac{b^3 - a^3}{3} - (a+b)\frac{(b^2 - a^2)}{2} + ab(b-a)$$

$$= (b-a)\left[\frac{(b^2 + ab + a^2)}{3} - \frac{(a+b)^2}{2} + ab\right]$$

$$= -\frac{(b-a)^3}{6}.$$

Let $n=2$. Then

$$f(x) = P_2(x) + f[x_0, x_1, x_2, x]\, \psi_2(x). \qquad \psi_2(x) = \prod_{j=0}^{2}(x-x_j)$$

Note for distinct x_0, x_1, x_2 in $[a,b]$,

$\psi_2(x) = (x-x_0)(x-x_1)(x-x_2)$ is not of one sign on (a,b). But if we choose $x_0=a$, $x_1=(a+b)/2$, $x_2=b$, then we can show that

$$\int_a^b \psi_2(x)\,dx = \int_a^b (x-a)\left(x-\left(\tfrac{a+b}{2}\right)\right)(x-b)\,dx = 0.$$

Let $x = a+(b-a)\hat{x}$, $\hat{x}\in[0,1]$

then $\hat{x}=0 \Rightarrow x=a$;
$\hat{x}=1 \Rightarrow x=b$;

$dx = (b-a)\,d\hat{x}$
$x-a = (b-a)\hat{x}$
$x-b = (b-a)(\hat{x}-1)$
$x-\left(\frac{a+b}{2}\right) = (b-a)(\hat{x}-1/2)$

$$\int_a^b \psi_2(x)\,dx = \int_0^1 \hat{x}(\hat{x}-1)(\hat{x}-1/2)(b-a)^4\,d\hat{x}.$$

$$= \frac{(b-a)^4}{2}\int_0^1 \hat{x}(\hat{x}-1)(2\hat{x}-1)\,d\hat{x}$$

$$= \cancel{\frac{(b-a)}{2}}\ \frac{(b-a)^4}{2}\int_0^1 (\hat{x}^2-\hat{x})(2\hat{x}-1)\,d\hat{x}$$

$$= \frac{(b-a)^4}{2}\int_0^1 (2\hat{x}^3-\hat{x}^2-2\hat{x}^2+\hat{x})\,d\hat{x}$$

$$= \frac{(b-a)^4}{2}\left[\frac{2\hat{x}^4}{4} - \hat{x}^3 + \frac{\hat{x}^2}{2}\right]_{\hat{x}=0}^{\hat{x}=1}$$

$$= \frac{(b-a)^4}{2}\left[\tfrac{1}{2}-1+\tfrac{1}{2}\right] = 0.$$

The error is of the form (3). If we choose

$x_3 = x_1 = (a+b)/2$. then

$$\psi_3(x) = (x-a)\left(x-\frac{a+b}{2}\right)^2(x-b)$$

is of one sign on (a,b)

Hence

$$I(f) = I(p_2) + \frac{1}{4!} f^{(4)}(\eta) \int_a^b \psi_3(x)\,dx, \quad \eta \in (a,b).$$

we can calculate

$$\int_a^b \psi_3(x)\,dx = \int_a^b (x-a)\left(x-\frac{a+b}{2}\right)^2 (x-b)\,dx$$

$$= \frac{(b-a)^5}{4} \int_0^1 \hat{x}(\hat{x}-1)(2\hat{x}-1)^2\,d\hat{x}$$

$$= \frac{(b-a)^5}{4} \int_0^1 (\hat{x}^2-\hat{x})(4\hat{x}^2+1-4\hat{x})\,d\hat{x}$$

$$= \frac{(b-a)^5}{4} \int_0^1 \left[4\hat{x}^4+\hat{x}^2-4\hat{x}^3-4\hat{x}^3-\hat{x}+4\hat{x}^2\right] d\hat{x}$$

$$= \frac{(b-a)^5}{4} \int_0^1 \left[4\hat{x}^4+5\hat{x}^2-8\hat{x}^3-\hat{x}\right] d\hat{x}$$

$$= \frac{(b-a)^5}{4} \left[4\frac{\hat{x}^5}{5}+\frac{5\hat{x}^3}{3}-\frac{8\hat{x}^4}{4}-\frac{\hat{x}^2}{2}\right]_{\hat{x}=0}^{1}$$

$$= \frac{(b-a)^5}{4}\left[\frac{4}{5}+\frac{5}{3}-2-\frac{1}{2}\right] = \frac{(b-a)^5}{4}\cdot\left(-\frac{1}{30}\right)$$

$$= -\frac{4}{15}\left(\frac{b-a}{2}\right)^5.$$

So that the error for this formula becomes

$$E^S(f) = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\eta), \quad \eta \in (a,b).$$

We now calculate $I(P_2)$ to obtain the formula:

Since $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$. The interpolating polynomial P_2 is given by

$$P_2(x) = f(a) + f[a,b](x-a) + f\left[a,b,\tfrac{a+b}{2}\right](x-a)(x-b)$$

Then

$$\int_a^b P_2(x)\,dx = f(a)(b-a) + f[a,b]\frac{(b-a)^2}{2} + f\left[a,b,\tfrac{a+b}{2}\right]\cdot \int_a^b (x-a)(x-b)\,dx.$$

Note that $\int_a^b (x-a)(x-b)\,dx = -\frac{(b-a)^3}{6}$. We note that

$$\int_a^b P_2(x)\,dx = f(a)(b-a) + f[a,b]\frac{(b-a)^2}{2} - f\left[a,b,\tfrac{a+b}{2}\right]\frac{(b-a)^3}{6}.$$

$$= (b-a)\left[f(a) + f[a,b]\frac{(b-a)}{2} - f\left[a,b,\tfrac{a+b}{2}\right]\frac{(b-a)^2}{6}\right]$$

We know $f\left[a,b,\tfrac{a+b}{2}\right] = f\left[a,\tfrac{a+b}{2},b\right]$

$$f\left[a,\tfrac{a+b}{2},b\right](b-a)^2 = \left\{f\left[\tfrac{a+b}{2},b\right] - f\left[a,\tfrac{a+b}{2}\right]\right\}(b-a)$$

$$= \frac{f(b) - f\left(\frac{a+b}{2}\right) - f\left(\frac{a+b}{2}\right) + f(a)}{\frac{(b-a)}{2}}(b-a)$$

$$= 2\left\{f(b) + f(a) - 2f\left(\tfrac{a+b}{2}\right)\right\}$$

$$\therefore \int_a^b P_2(x)\,dx = (b-a)\left[f(a) + (f(b)-f(a))/2 - \frac{2}{6}\left(f(b)+f(a)-2f\left(\tfrac{a+b}{2}\right)\right)\right]$$

$$= \frac{(b-a)}{6}\left[f(a) + 4f\left(\tfrac{a+b}{2}\right) + f(b)\right]$$

$$\boxed{I(f) \approx S = \frac{b-a}{6}\left[f(a) + 4f\left(\tfrac{a+b}{2}\right) + f(b)\right].}$$