$$\Rightarrow \frac{f(x+h)-f(x)}{h} = f'(x) + \underbrace{\frac{f''(x)}{2!}h + \frac{f'''(x)}{3!}h^2 + \cdots}_{\text{If } h \text{ is small, truncate}}$$

$$\Rightarrow \boxed{f'(x) \approx \frac{f(x+h)-f(x)}{h} \quad \text{with approximation error } O(h)}$$

Backward Difference Approximation

Use B series

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \cdots$$

$$\frac{f(x)-f(x-h)}{h} = f'(x) - \underbrace{\frac{f''(x)}{2!}h + \frac{f'''(x)}{3!}h^2 + \cdots}_{h \text{ small} \Rightarrow \text{truncate}}$$

$$\Rightarrow \boxed{f'(x) \approx \frac{f(x)-f(x-h)}{h} \quad \text{with approx. error } O(h)}$$

Centered Difference (1st Derivative)

Use (A) − (B):

$$f(x+h) = f(x) + f'(x)\cdot h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \cdots$$

$$f(x-h) = f(x) - f'(x)\,h + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \cdots$$

Subtract:

$$f(x+h) - f(x-h) = 2f'(x)\,h + 2\,\frac{f'''(x)}{3!}\,h^3 + \cdots$$

$$\Rightarrow \frac{f(x+h) - f(x-h)}{2h} = f'(x) + \underbrace{\frac{f'''(x)}{3!}\,h^2 + \cdots}_{h \text{ small } \Rightarrow \text{ truncate}}$$

$$\Rightarrow \boxed{f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \quad \text{with approx. error } O(h^2)}$$

Remarks:

1) Typically used for tabulated data $\{(x_i, f_i)\}_{i=1}^{n}$ or solving differential eqns. Else, can use symbolic $f'(x)$

2) Want h sufficiently small, but not so small as to lead to cancellation of significant digits. $(f(x+h) - f(x))$

- One remedy: centered differences

3) In practice, if h is much smaller than $\sqrt{\varepsilon}$, round-off errors will dominate

machine epsilon

Double precision: $\sqrt{\varepsilon_D} \approx 10^{-8}$

Single precision: $\sqrt{\varepsilon_S} \approx 10^{-4}$

Centered Difference (2nd Derivative)

Use A + B :

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \cdots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \cdots$$

$$\Rightarrow f(x+h) + f(x-h) = 2f(x) + f''(x)h^2 + \frac{2f^{(4)}(x)}{4!}h^4 + \cdots$$

$$\Rightarrow \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \underbrace{\frac{2f^{(4)}(x)}{4!} \cdot h^2 + \cdots}_{h \text{ small} \Rightarrow \text{truncate}}$$

$$\Rightarrow \boxed{f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \quad \text{with approx. error } O(h^2)}$$

Ex: Poisson's Eqn. in one dimension.

$$-\frac{d^2u(x)}{dx^2} = f(x) \qquad 0 < x < 1 \qquad \text{(D.E.)}$$

where $f(x)$ is given, $u(x)$ is unknown.

Assume Dirichlet Boundary Conditions:

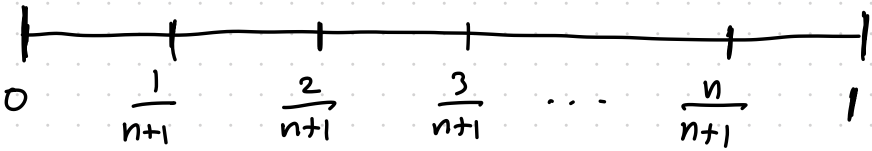
$$u(0) = 0 = u(1)$$

One approach to solve (D.E): Discretize and use linear algebra.

That is,

- Try to compute an approximate solution at $n+2$ equally spaced points, x_i

$$x_i = i \cdot h \,, \quad h = \frac{1}{n+1} \,, \qquad 0 \le i \le n+1$$



- Denote $u_i = u(x_i)$ and $f_i = f(x_i)$

- Try to D.E. to a linear system using finite difference approx.

$$\frac{d^2u(x)}{dx^2} \approx \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

$$= \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2}$$

$$= \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

∴ Poisson Eqn. $-\frac{d^2 u}{dx^2} = f(x)$ gives

approximation:

$$\frac{-u_{i-1} + 2u_i - u_{i+1}}{h^2} = f_i, \quad i = 1, 2, \ldots, n$$

or $-u_{i-1} + 2u_i - u_{i+1} = h^2 f_i, \quad i = 1, 2, \ldots, n.$

- Since the boundary conditions imply

$u_0 = u_{n+1} = 0$, we can obtain the system of

eqns:

$$\begin{array}{ll}
i=1: & 2u_1 - u_2 = h^2 f_1 \\
i=2: & -u_1 + 2u_2 - u_3 = h^2 f_2 \\
i=3: & -u_2 + 2u_3 - u_4 = h^2 f_3 \\
\vdots & \\
i=n-1 & -u_{n-2} + 2u_{n-1} - u_n = h^2 f_{n-1} \\
i=n & -u_{n-1} + 2u_n = h^2 f_n
\end{array}$$

$$\Rightarrow \begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} = h^2 \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}$$

100

$$\Rightarrow A\underline{u} = \underline{b}$$

$$\Rightarrow \underline{u} = A \backslash \underline{b}$$

Numerical Integration

Basic Idea:

- approx. $f(x)$ by polynomial $p(x)$
- Then

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

That, the quadrature rule is

$$R(f) = \int_a^b p(x)\,dx$$

- Using Lagrange form of $p(x)$, we get

$$\boxed{\begin{aligned} R(f) &= \sum_{i=0}^{n} w_i\, f(x_i) \\ \text{where} \quad w_i &= \int_a^b L_{n,i}(x)\,dx \end{aligned}}$$

Note:

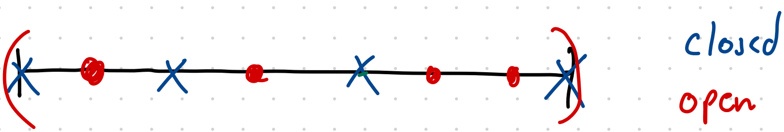
$$\int_a^b p(x)\,dx = \int_a^b \sum_{i=0}^{n} L_{n,i}(x)\cdot f(x_i)\,dx$$

$$= \sum_{i=0}^{n} \underbrace{\int_a^b L_{n,i}(x)\,dx}_{w_i}\, f(x_i)$$

When nodes are equally spaced, we obtain the Newton-Cotes (NC) formulae:

Closed NC rule: include boundary points $[a,b]$

Open NC rule: exclude boundary points (a,b)



Ex: $n=2$ (degree 1 poly) using $x_0=a$, $x_1=b$ (closed)

$p(x)$

$$R(f) = \sum_{i=0}^{1} w_i f(x_i) = w_0 f(x_0) + w_1 f(x_1)$$

$$= w_0 f(a) + w_1 f(b)$$

where $w_i = \int_a^b L_{n,i}(x)\,dx$, $i=0,1$

$$w_0 = \int_a^b L_{1,0}(x)\,dx = \int_a^b \frac{(x-b)}{(a-b)}\,dx = \frac{b-a}{2}$$

$$w_1 = \int_a^b L_{1,1}(x)\,dx = \int_a^b \frac{(x-a)}{(b-a)}\,dx = \frac{b-a}{2}$$

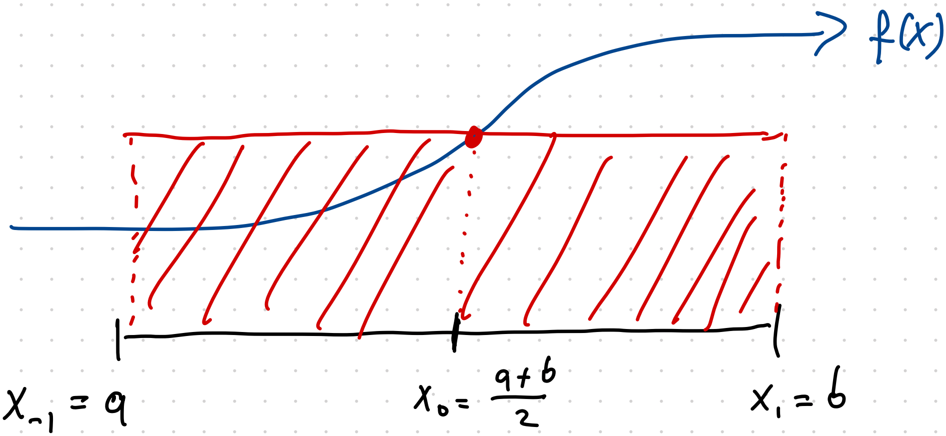
$$\Rightarrow \boxed{R(f) = \frac{b-a}{2}\left(f(a)+f(b)\right)} \leftarrow \text{Trapezoidal Rule!}$$

More generally:

- **Midpoint Rule** (open 1-point NC rule)

$$R(f) = (b-a)\cdot f\left(\frac{a+b}{2}\right) = (x_1 - x_{-1})\cdot f(x_0)$$

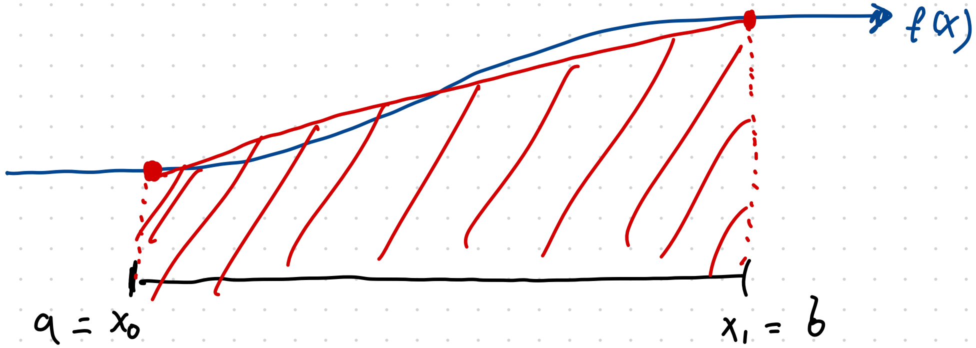
$\Rightarrow$ $p(x)$ has degree 0 (i.e., interpolate using constant func.)



- **Trapezoidal Rule** (closed 2-point NC Rule)

$$R(f) = \frac{b-a}{2}\left(f(a)+f(b)\right) = \frac{\overbrace{x_1-x_0}^{h}}{2}\left(f(x_0)+f(x_1)\right)$$

$\Rightarrow p(x)$ has degree 1 (i.e., interpolate using linear function)

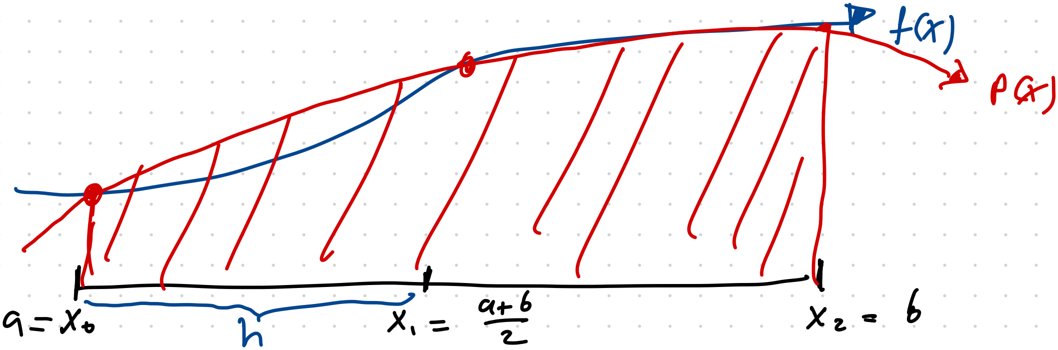


- **Simpson's $\frac{1}{3}$ Rule** (closed 3-pt. NC Rule)

$$R(f) = \frac{b-a}{6}f(a) + \frac{2(b-a)}{3}f\left(\frac{a+b}{2}\right) + \frac{b-a}{6}f(b)$$

$$= \frac{h}{3}f(x_0) + \frac{4h}{3}f(x_1) + \frac{h}{3}f(x_2) \qquad \left(h = \frac{b-a}{2}\right)$$

$\Rightarrow p(x)$ has degree 2 (interpolate with quadratic



Degree of Precision (DOP)

$(R(f) = I(f))$

If a quadrature rule $R(f) = \sum_{i=0}^{n} w_i f(x_i)$ exactly integrates all polynomials of degree $\leq m$, then we say that $R(f)$ has DOP m

Note: To find DOP, we only need to check

$$R(f) \overset{?}{=} \int_a^b 1\,dx$$

$$R(f) \overset{?}{=} \int_a^b x\,dx$$

$$\vdots$$

$$R(f) \overset{?}{=} \int_a^b x^m\,dx$$

Remark: For interpolatory quadrature,

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

is constructed so that $R(f) = \int_a^b p(x)\,dx$, where $p(x)$ is a polynomial of fixed degree.

Thus, if $p(x)$ has degree m, then DOP $\geq m$

Can DOP $> m$?

Ex: Find DOP for midpoint rule:

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

- $f(x) = 1 \implies f\left(\frac{a+b}{2}\right) = 1$

$$\implies R(f) = (b-a) \cdot 1 = b-a$$

$$\int_a^b 1\,dx = x\Big|_a^b = b-a$$

same!

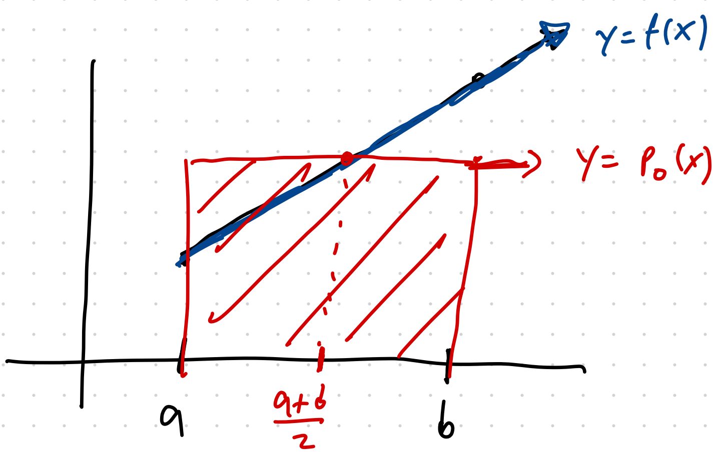
- $f(x) = x \implies f\left(\frac{a+b}{2}\right) = \frac{a+b}{2}$

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

$$\int_a^b x\,dx = \frac{1}{2}x^2\Big|_a^b$$

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

same!



- $f(x) = x^2 \Rightarrow f\left(\frac{a+b}{2}\right) = \frac{(a+b)^2}{4}$

$$\Rightarrow R(f) = (b-a)\frac{(a+b)^2}{4}$$

$$\int_a^b x^2 dx = \frac{x^3}{3}\Big|_a^b = \frac{1}{3}\left[b^3 - a^3\right]$$

NOT the same!

$$\Rightarrow \boxed{\text{Midpoint Rule DOP} = 1}$$

Note: Midpt. Rule is interpolatory quad. rule using degree $m=0$ poly.

BUT $\quad$ DOP $= m+1 = 1$

Ex: Find DOP of Trap. Rule.

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

We know

$$R(1) = \int_a^b 1\,dx$$

$$R(x) = \int_a^b x\,dx$$

no need to check these

So DOP is at least 1. $\quad$ Check: $R(x^2) \overset{?}{=} \int_a^b x^2 dx$

- $f(x) = x^2 \Rightarrow f(a) = a^2, \; f(b) = b^2$

$$\Rightarrow R(f) = \frac{b-a}{2}(a^2+b^2)$$

$$\int_a^b x^2 dx = \frac{1}{3}x^3 \Big|_a^b = \frac{1}{3}(b^3 - a^3)$$

NOT the same!

$\Rightarrow$ $\boxed{\text{Trap. Rule has DOP} = 1}$

Note: Trap. Rule is an interpolatory quad. rule using degree $m=1$ poly., and

$$\text{DOP} = m = 1$$

Ex: Simpson's $\frac{1}{3}$ Rule

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

We know:

$$\left.\begin{aligned} R(1) &= \int_a^b 1\, dx \\ R(x) &= \int_a^b x\, dx \\ R(x^2) &= \int_a^b x^2 dx \end{aligned}\right\} \text{no need to check these}$$

Check: $R(x^3) \overset{?}{=} \int_a^b x^3\,dx$

- $f(x) = x^3 \Rightarrow f(a) = a^3,\ f\left(\frac{a+b}{2}\right) = \frac{(a+b)^3}{8},\ f(b) = b^3$

$$\Rightarrow R(f) = \frac{b-a}{6}\left(a^3 + \frac{4(a+b)^3}{8} + b^3\right)$$

$$= \cdots = \frac{1}{4}\left(b^4 - a^4\right)$$

$$\int_a^b x^3\,dx = \frac{1}{4}x^4\Big|_a^b = \frac{1}{4}\left(b^4 - a^4\right)$$

Same!

Check: $R(x^4) = \int_a^b x^4\,dx$.

Can show $R(x^4) \neq \int_a^b x^4\,dx$

$\Rightarrow$ $\boxed{\text{Simpson's } \tfrac{1}{3} \text{ Rule DOP} = 3}$

Note: Simpson's $\frac{1}{3}$ Rule is an interp. quad. rule using deg. $m = 2$ polynomial,

BUT DOP $= m+1 = 3$

<u>Remark:</u> This pattern is true in general.
That is, for intep. quadrature rule with equally-space points (NC-rules),

- If degree $\deg.(p(x)) = m$ is odd, then $R(f)$ has $DOP = m$
- If degree $\deg(p(x)) = m$ is even, then $R(f)$ has $DOP = m+1$.

Closed-NC Error Thm: Suppose $R(f) = \sum_{i=0}^{n} w_i f(x_i)$ denotes the $(n+1)$-closed NC rule with $x_0 = a$, $x_n = b$, $h = \frac{b-a}{n}$. Then there exists $\xi \in (a,b)$ s.t.

- When n is even and $f \in C^{(n+2)}(a,b)$

$$\int_a^b f(x)\,dx = R(f) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)\,dt$$

- When n is odd and $f \in C^{(n+1)}(a,b)$

$$\int_a^b f(x)\,dx = R(f) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)\,dt$$

<u>Note:</u> n even $\Rightarrow O(h^{n+3})$ error

n odd $\Rightarrow O(h^{n+2})$ error