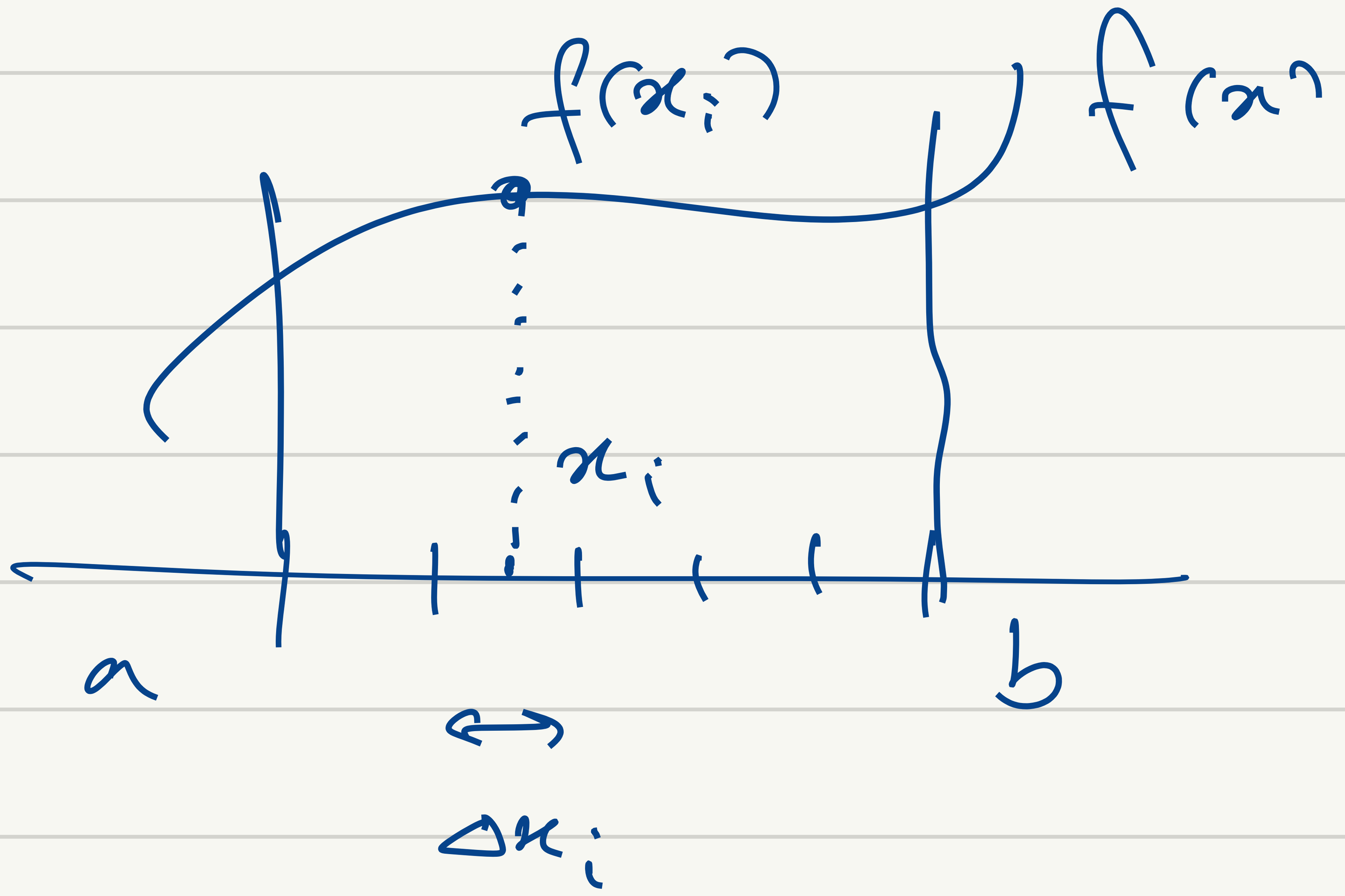
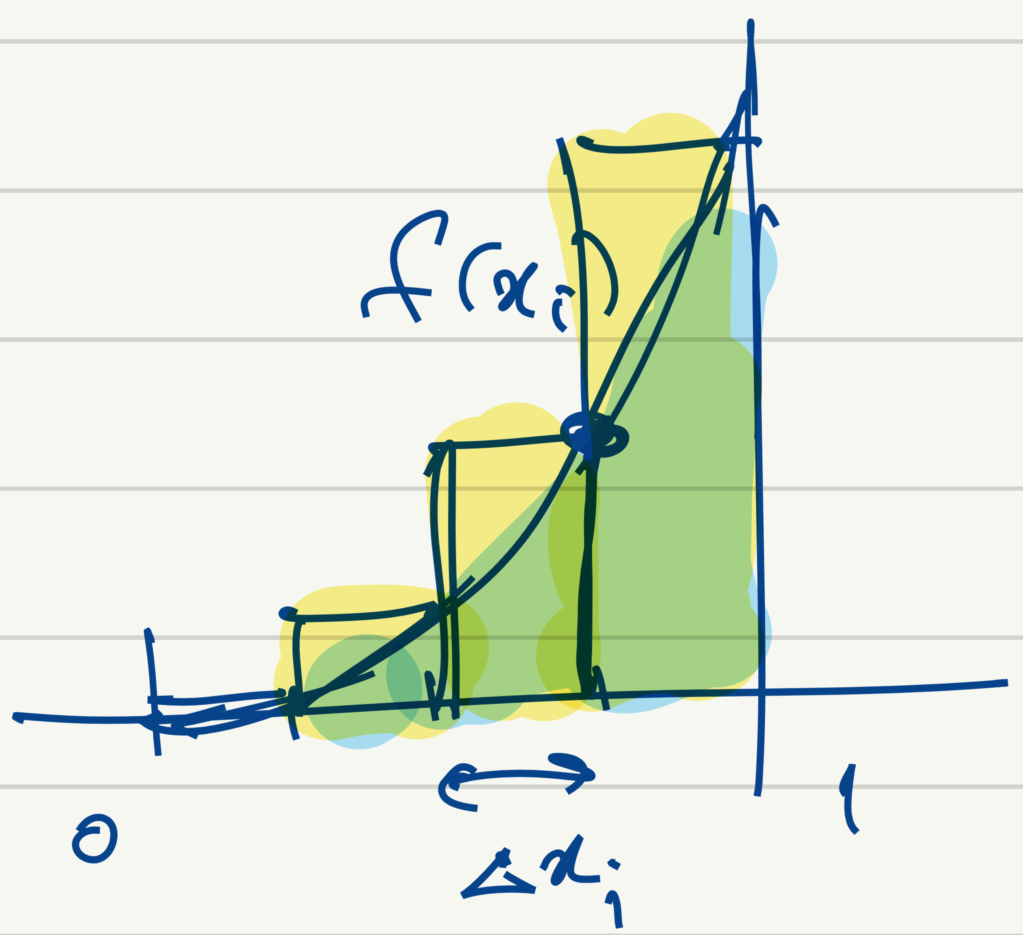
Numerical Integration

$\rightarrow \boxed{f} \rightarrow \quad , \quad [a,b] \quad \rightarrow \quad I(f) = \int_a^b f(x)\,dx = \lim_{\substack{n\to\infty \\ \max \Delta x_i \to 0}} \sum_{i=1}^{n} f(x_i)\,\Delta x_i$

Riemann sum: $\sum_{i=1}^{n} \underbrace{f(x_i)\,\Delta x_i}$

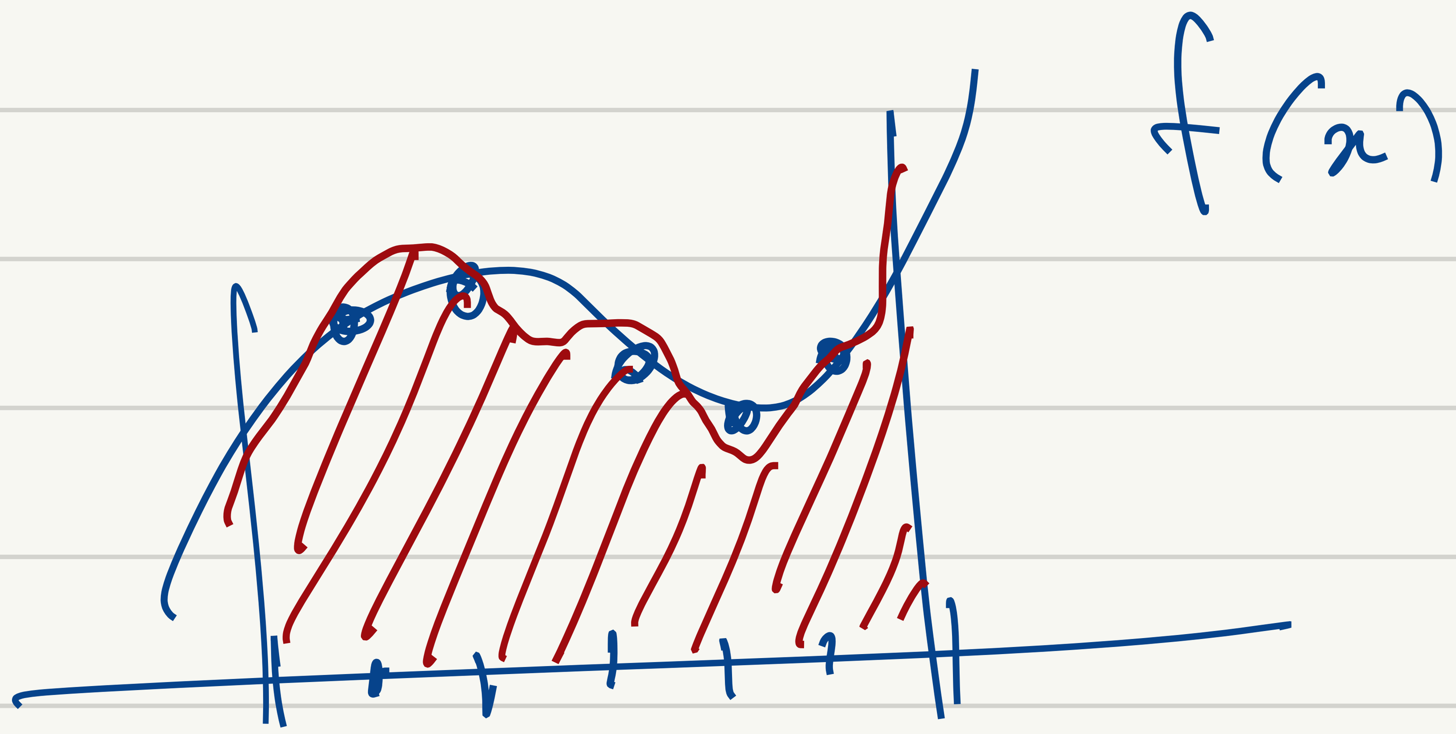




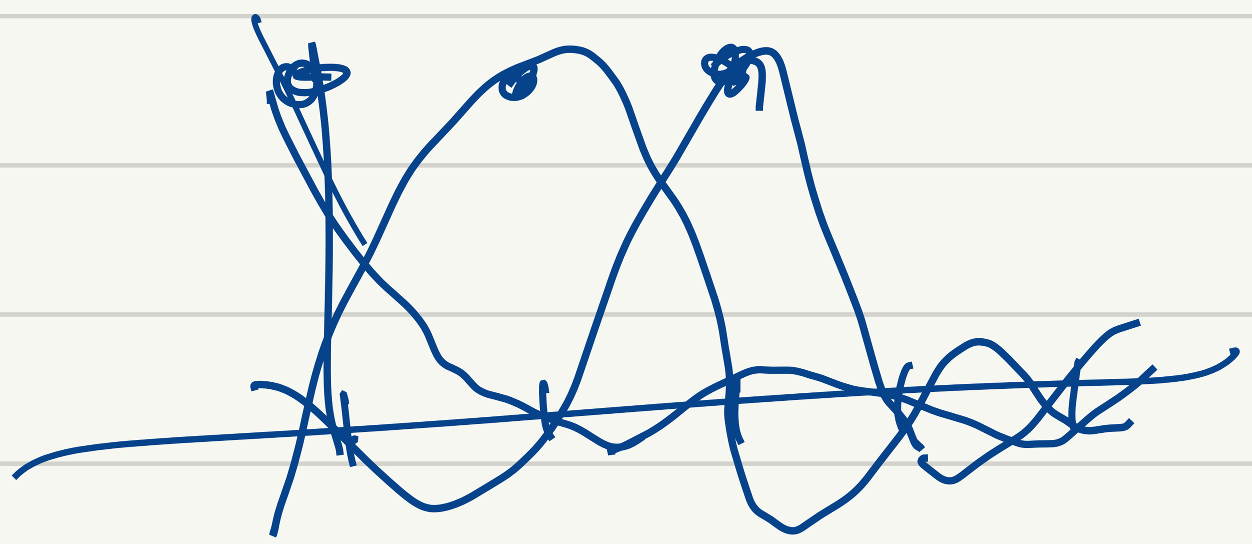
$f(x) = x^2 \qquad I(f) = 1/3$

$x_i = \frac{i}{n} \;,\; \Delta x = \frac{1}{n} \;\rightarrow\; \sum \left(\frac{i}{n}\right)^2 \cdot \frac{1}{n} = \frac{1}{3} + O\left(\frac{1}{n}\right)$

Integral of approx. of f = approx. of integral of f.



$$x_i,\ f(x_i) \longrightarrow p(x)$$

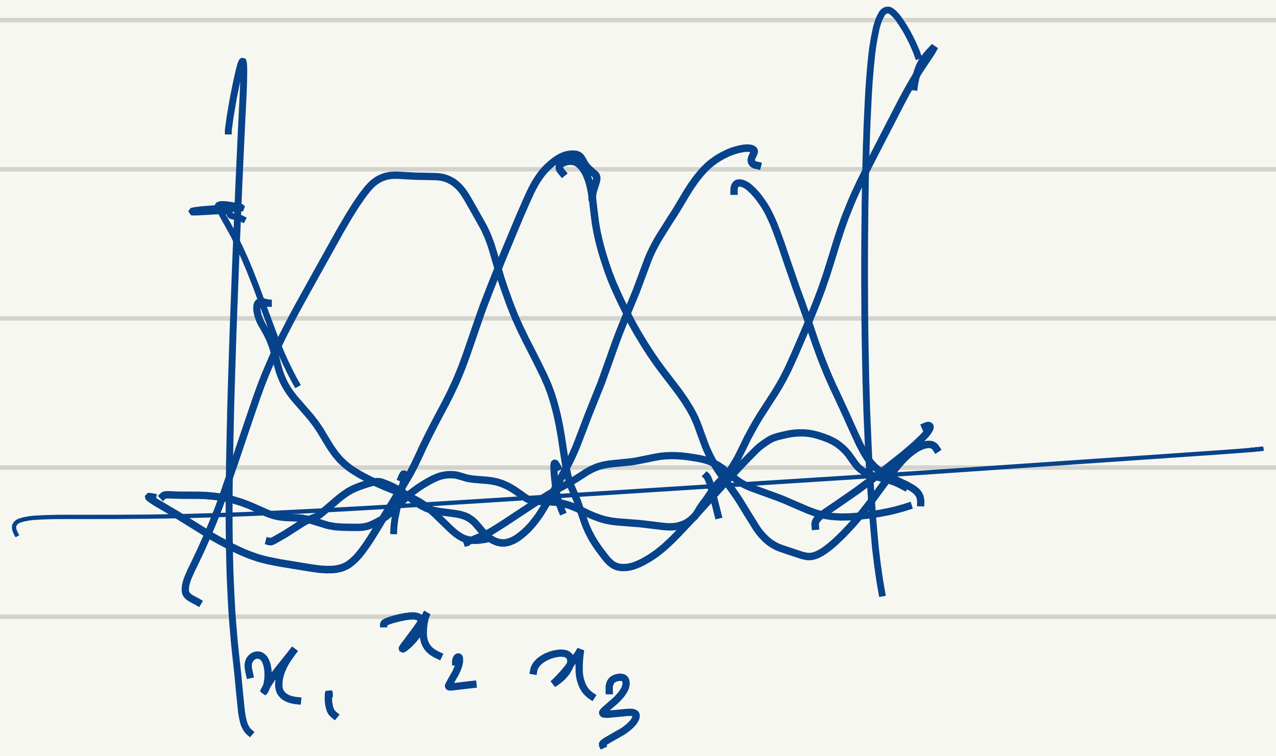


$$\boxed{\begin{aligned} p &= \sum_{i=1}^{n} c_i \phi_i \\ &= \sum_{i=1}^{n} f(x_i)\, l_i \end{aligned}}$$

in Lagrange basis

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

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



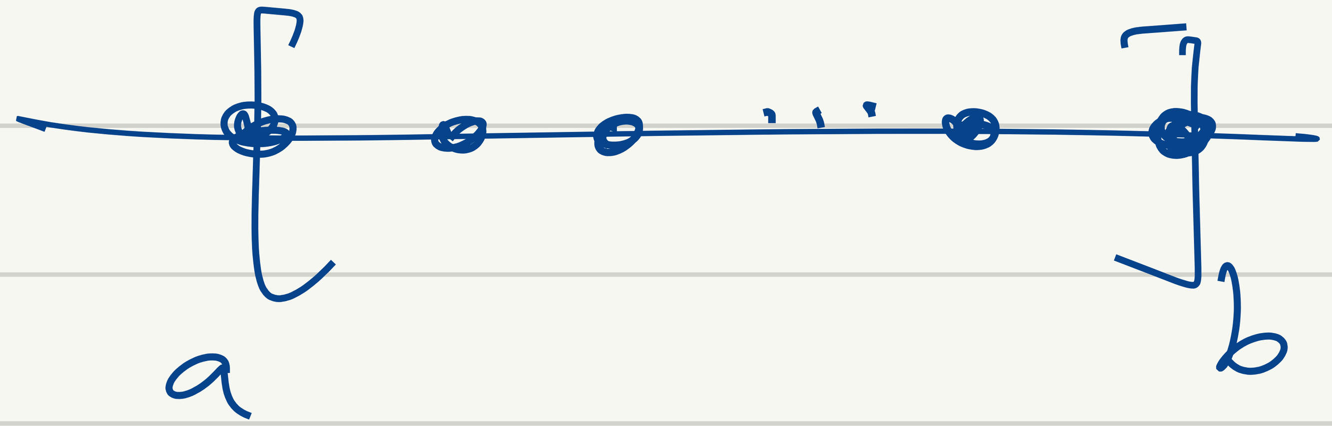
$$= \sum_{i=1}^{n} f(x_i) \underbrace{\int_a^b l_i(x)\, dx}_{w_i}$$

$$= \boxed{\sum_{i=1}^{n} w_i f(x_i)}$$

$$\boxed{Q_n(f) = \sum_{i=1}^{n} w_i \, f(x_i)} \quad : \quad n\text{-point } \boxed{\text{quadrature rule}}$$

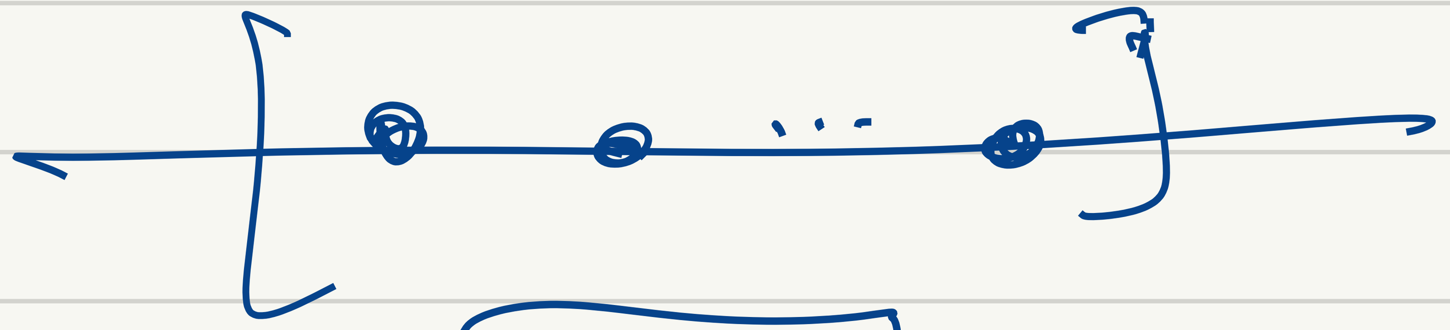
w_i: **weights** or **coefficients**

x_i: **nodes** or **abscissas** or **quadrature points**



closed q.r.

If w_i from interpolation: **interpolatory** q.r.



open q.r.

1. How to choose nodes x_i
2. How to choose weights w_i

} so that $Q_n(f)$ is close to $I(f)$

3. How to quantify closeness?

Let's say we've fixed $x_1, x_2, \dots, x_n$

- $l_i(x) = \dfrac{\prod_{j \neq i} (x - x_j)}{\prod_{j \neq i} (x_i - x_j)}$, $w_i = \int_a^b l_i(x)\, dx$

- find w_i so that $Q_n(p) = I(p)$ for all degree $n-1$ polynomials

$$\left.\begin{aligned} \Sigma w_i = \Sigma w_i x_i^0 &= \int_a^b x^0\, dx = b-a \\ \Sigma w_i x_i &= \int_a^b x\, dx \\ &\vdots \\ \Sigma w_i x_i^{n-1} &= \int_a^b x^{n-1}\, dx \end{aligned}\right\} \text{closed form}$$

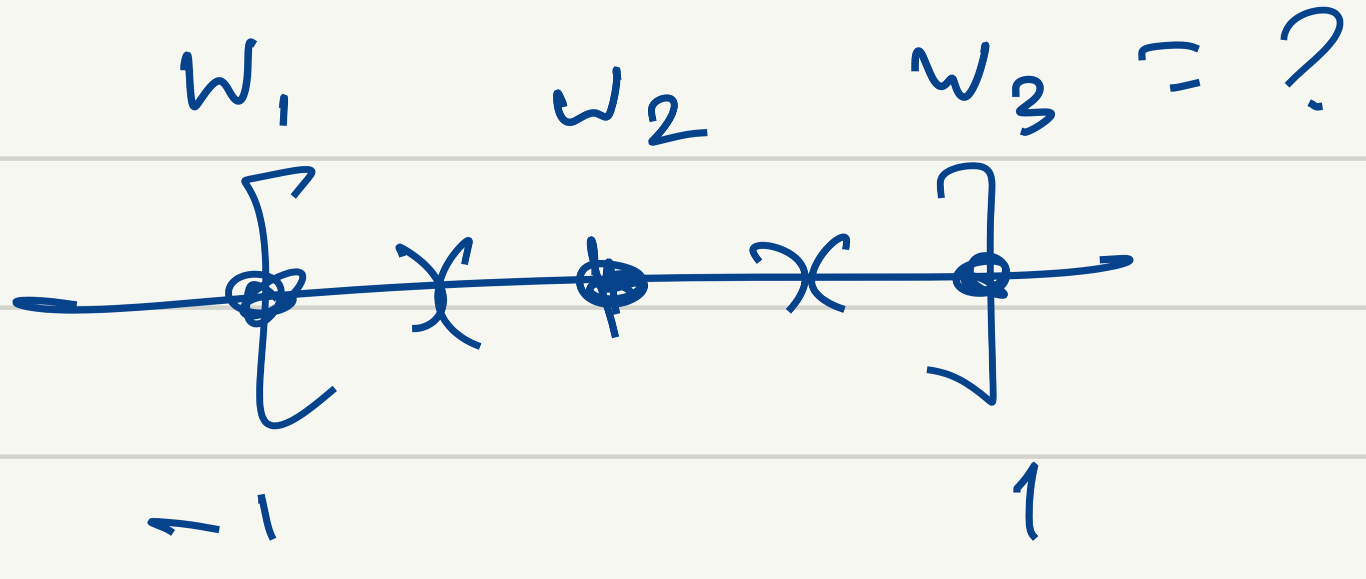
$A\vec{w}$ $\vec{b}$

$\boxed{\text{moment equations}}$

$\boxed{\text{method of undetermined coefficients}}$

$\Sigma w_i = b-a$

Example:



$\vec{w} = [2/3,\ 2/3,\ 2/3]$?

$\vec{w} = [1/2,\ 1,\ 1/2]$?

$$\begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 2/3 \end{bmatrix} \longrightarrow \vec{w} = [1/3,\ 4/3,\ 1/3] \ : \text{degree} \geq 2$$

$Q(ax^2 + bx + c) =$

- Divided differences.

(more numerically stable)

Accuracy: $\boxed{\text{Degree}}$ of quadrature rule = largest d s.t. $Q_n(p) = I(p)$ for all degree-d polynomials p

Interpolatory q.r. on n points $\iff$ degree $\geq n-1$

for arbitrary f, how close are $I(f)$ and $Q_n(f)$?

p_{n-1} : interpolating polynomial $\Rightarrow$ $p_{n-1}(x_i) = f(x_i)$

$$Q_n(f) = I(p_{n-1})$$

$$|I(f) - Q_n(f)| = |I(f) - I(p_{n-1})|$$
$$= |I(f - p_{n-1})| \leq (b-a) \underbrace{\|f - p_{n-1}\|}$$

~~bounds~~ bounds from prev. chapter. depends on $\|f^{(n)}\|$

<u>Stability</u> : Suppose $\tilde{f}(x_i) = f(x_i) + \delta f(x_i)$,

$$\|\delta f\| \leq \varepsilon$$

change in $Q_n(f)$: $|Q_n(\tilde{f}) - Q_n(f)| = |Q_n(\delta f)| = \left|\sum_{i=1}^{n} w_i \, \delta f(x_i)\right|$

$$\leq \left(\sum |w_i|\right) \underbrace{\|\delta f\|}_{\leq \varepsilon}$$

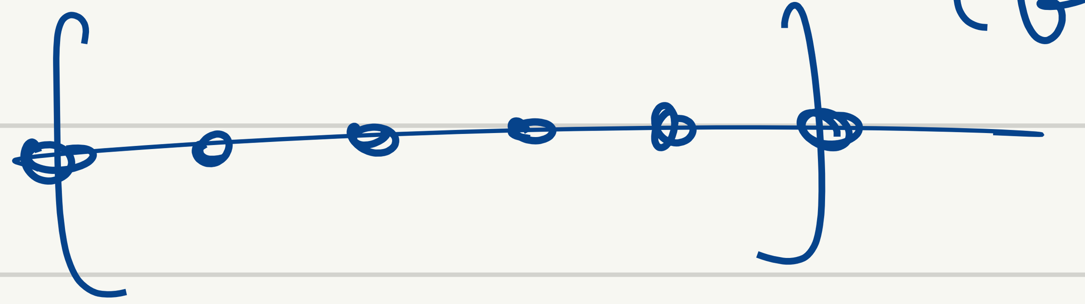
$$|I(f+\delta f) - I(f)| \le \underbrace{(b-a)\,\|\delta f\|}$$

Recall $\sum w_i = b-a$

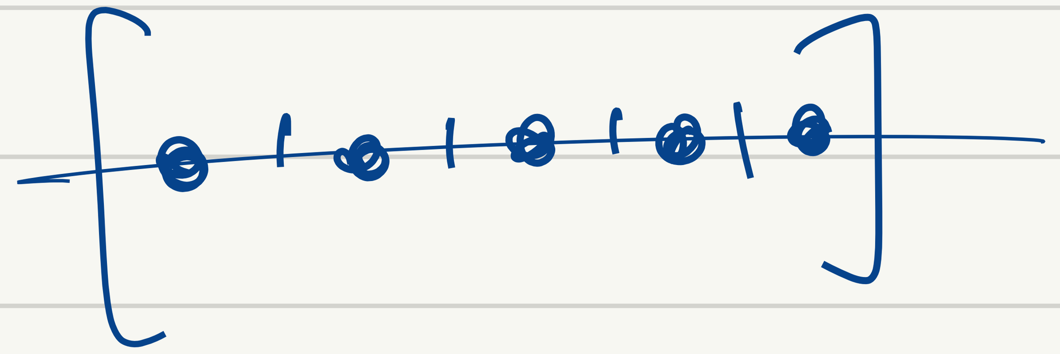
1. if $w_i \ge 0$ then $\sum |w_i| = \sum w_i = b-a \Rightarrow$ stable
2. if some $w_i < 0$ then $\sum |w_i|$ could be $\gg b-a \Rightarrow$ unstable

---

Newton-Cotes quadrature : equally spaced x_i



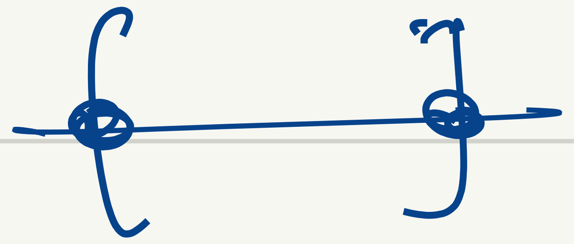
closed

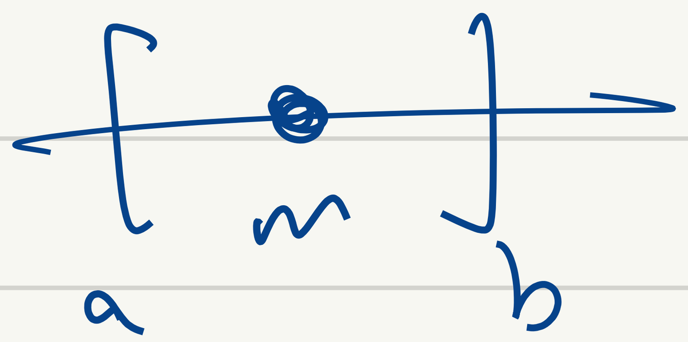


open

1. 1-point open : midpoint rule $M(f) = (b-a)\,f(m)$

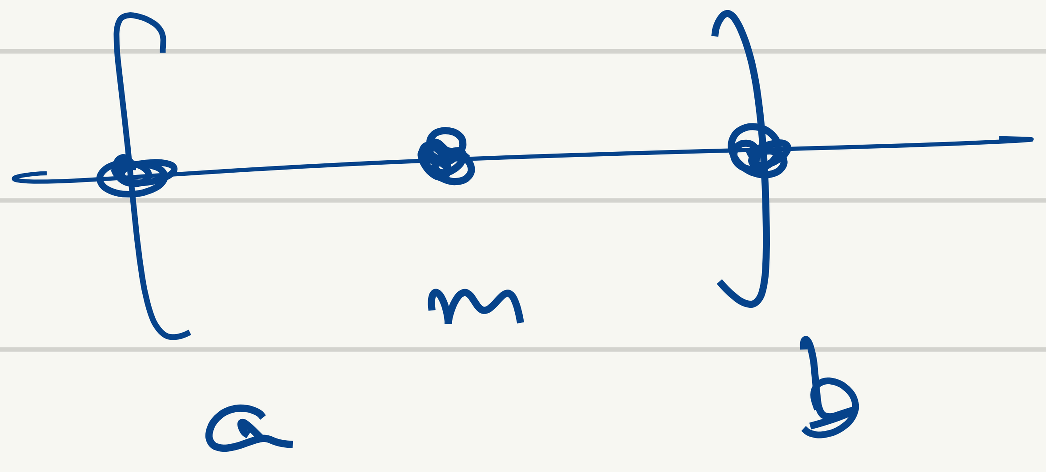
2-point closed : trapezoidal rule





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

3-point closed



Simpson's rule $S(f) = \frac{b-a}{6}\left(f(a) + 4(m) + f(b)\right)$

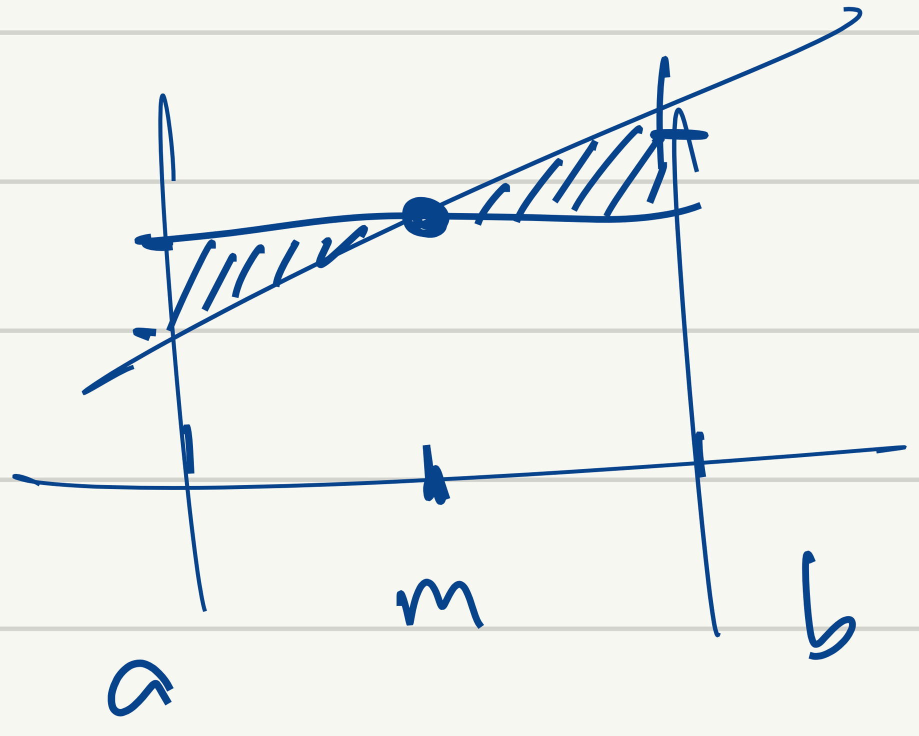
Error analysis

Taylor series $f(x) = f(m) + \underbrace{f'(m)(x-m)} + \frac{f''(m)}{2}(x-m)^2 + \frac{f'''(m)}{6}(x-m)^3 + O((x-m)^4)$

$I(f) = f(m)(b-a) + 0 + \frac{f''(m)}{24}(b-a)^3 + O((b-a)^5)$

$M(f) = f(m)(b-a) \implies$ error in midpoint rule $= \frac{f''(m)}{24}(b-a)^3 + O((b-a)^5)$

Similarly, $I(f) - T(f) = -\frac{f''(m)}{12}(b-a)^3 + O((b-a)^5)$



midpoint rule has degree 1 (not 0)

Same for odd n in Newton-Cotes: degree n

even n in Newton Cotes: degree $n-1$

Simpson's rule: $n=3$, degree $= 3$

for large n, instability due to Runge's phenomenon

for any $n \geq 11$, $\exists\, w_i < 0$, $\sum |w_i| \to \infty$ as $n \to \infty$

- Clenshaw-Curtis quadrature: Use x_i = Chebyshev points

$w_i > 0$, error $\to 0$ as $n \to \infty$

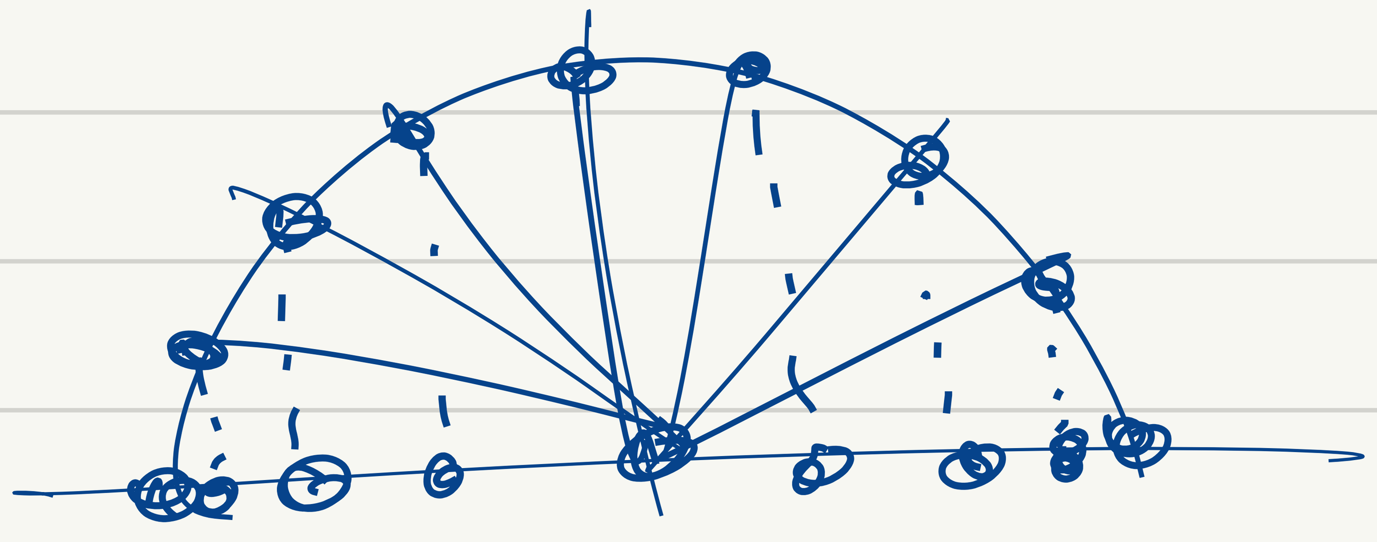
Compute w_i : - moment eqs.

- using fast fourier transform

Now can n large

Error estimate : $|Q_n(f) - Q_{2n}(f)|$

n nodes $2n$ nodes



5 → 9

points for $Q_{\sim 2n}$ ⊇ points for Q_n : $\boxed{\text{progressive}}$

q.v.

Gaussian quadrature

Treat x_i, w_i as variables!

2n variables $\Rightarrow$ match 2n equations $\Rightarrow$ degree $2n-1$ q.r.

$$\sum w_i = \int 1 \, dx$$

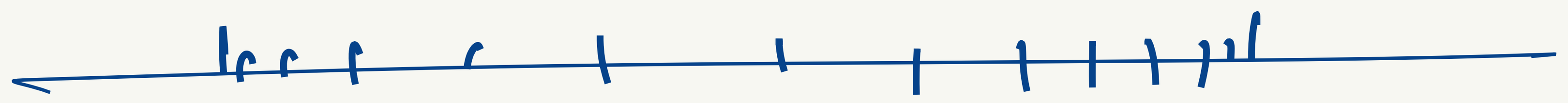
$$\sum w_i x_i = \int x \, dx$$

$$\sum w_i x_i^2 = \int x^2 \, dx$$

$$\vdots$$

$$\sum w_i x_i^{2n-1} = \int x^{2n-1} \, dx$$

Nodes x_i are roots of Legendre poly.



Theoretically optimal: highest degree possible with n nodes

In practice Clenshaw-Curtis is very close