

(forward/backward diff. quotient)

Taylor:

$$f(x+h) = f(x) + f'(x)h + \frac{f''(\xi)}{2} h^2$$

Rearrange:

$$\frac{f(x+h) - f(x)}{h} - f'(x) = \frac{f''(\xi)}{2} h$$

$\epsilon(h)$ think of this as a function of h that computes an approximation of $f'(x)$.

Then LHS is the error.

$$f(x-h) = f(x) - f'(x)h + \frac{f''(\hat{\xi})}{2} h^2$$

$$\frac{f(x) - f(x-h)}{h} - f'(x) = -\frac{f''(\hat{\xi})}{2} h$$

(centered difference quotient)

$$f(x+h) = f(x) + f'(x)h + \underbrace{f''(x)}_2 h^2 + \frac{f'''(\xi)}{6} h^3$$

$$f(x-h) = f(x) - f'(x)h + \underbrace{f''(x)}_2 h^2 - \frac{f'''(\xi)}{6} h^3$$

subtract and rearrange

$$\frac{f(x+h) - f(x-h)}{2h} - f'(x) = \frac{f''(\xi) + f''(\bar{\xi})}{2} h^2 - \frac{f'''(\xi)}{6} h^2.$$

$$\downarrow \quad \frac{f'''(\xi)}{6} h^2$$

Here, we used a little trick.

lemma : Let g is continuous on $[a,b]$.

Then, for any $x_1, x_2, \dots, x_n \in [a,b]$, there exists $\xi \in [a,b]$ such that

$$\text{mean} = \frac{g(x_1) + g(x_2) + \dots + g(x_n)}{n} = g(\xi) \dots (*)$$

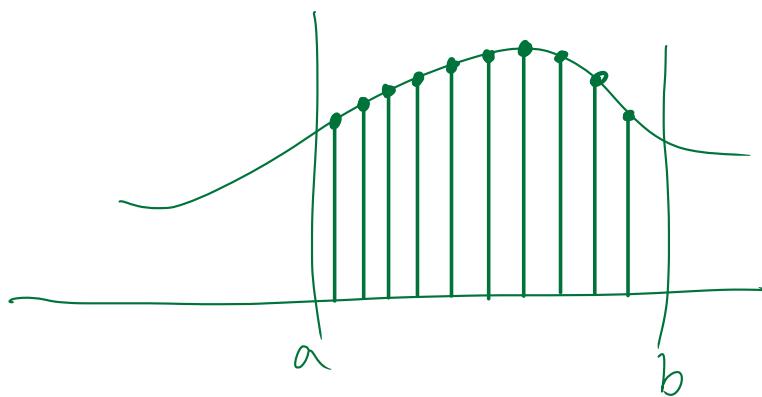
proof) The mean is b/w the maximum and the minimum of g over $[a,b]$. Hence, intermediate value theorem asserts that $\exists \xi$ satisfying $(*)$.

comment: This can be viewed as a discrete version of the mean value theorem of integral: If g is continuous,

$$\frac{1}{b-a} \int_a^b g(x) dx = g(\xi)$$

for some $\xi \in [a, b]$

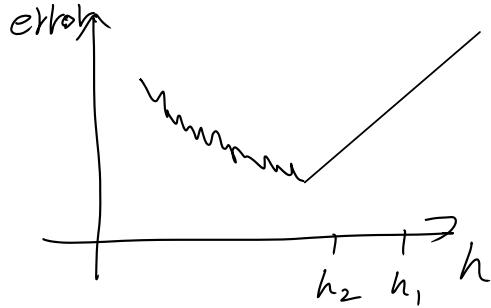
The LHS the mean of g using infinitely many samples.



$$\Delta x \approx \frac{b-a}{n} \Rightarrow \frac{1}{n} \approx \frac{\Delta x}{b-a}$$

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n g(x_i) &\approx \frac{1}{b-a} \sum_{i=1}^n g(x_i) \Delta x \\ &\approx \frac{1}{b-a} \int_a^b g(x) dx \end{aligned}$$

The slope of log-log scale is the rate of convergence.



spacing : $h_1 = 2h_2$ (h_1 : big, h_2 : small)

error : $e_1 \leftrightarrow h_1$, $e_2 \leftrightarrow h_2$

$$0 < \text{slope} = r = \frac{\Delta \log(\text{err})}{\Delta \log(\text{spacing})} = \frac{\log e_1 - \log e_2}{\log h_1 - \log h_2}$$

$$= \frac{\log \frac{e_1}{e_2}}{\log \frac{h_1}{h_2}} = \frac{\log e_1 / e_2}{\log 2}$$

$$\log e_1 / e_2 = r \log 2$$

$$\frac{e_1}{e_2} = e^{r \log 2} = 2^r$$

$$\frac{e_2}{e_1} = 2^{-r}$$

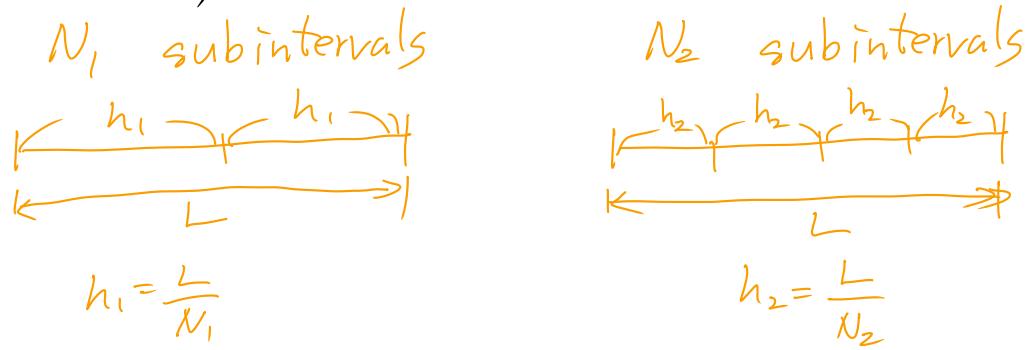
This is the general formula that works for any ratio of refinement, not necessarily $\frac{1}{2}$.

$$e_2 = 2^{-r} e_1 \rightarrow \text{half spacing} \rightarrow \text{half error}$$

If $r=1$, $e_2 = \frac{1}{2} e_1$
 If $r=2$, $e_2 = \frac{1}{4} e_1$
 half spacing \rightarrow a fourth error
 and so on.

If you use different resolutions instead of the spacing, you can modify the above formula to obtain the rate of convergence.

Suppose N_1 and N_2 correspond to h_1 and h_2 respectively.



From the general formula above

$$r = \frac{\log e_1/e_2}{\log h_1/h_2} = \frac{\log e_1/e_2}{\log \frac{L/N_1}{L/N_2}} = \frac{\log e_1/e_2}{\log N_2/N_1}.$$

$$f(x+h) = f(x) + f'(x)h + \underbrace{\frac{f''(x)}{2}h^2}_{\text{term}} + \underbrace{\frac{f'''(x)}{6}h^3}_{\text{term}} + \underbrace{\frac{f^{(4)}(x)}{24}h^4}_{\text{term}} + \dots$$

$$f(x-h) = f(x) - f'(x)h + \underbrace{\frac{f''(x)}{2}h^2}_{\text{term}} - \underbrace{\frac{f'''(x)}{6}h^3}_{\text{term}} + \underbrace{\frac{f^{(4)}(x)}{24}h^4}_{\text{term}} + \dots$$

subtract and rearrange:

$$\begin{aligned} (\ast) f'(x) &= \varphi(h) - \frac{f''(x)}{6}h^2 - \frac{f^{(5)}}{5!}h^4 - \dots \\ &= \varphi(h) - a_2 h^2 - a_4 h^4 - \dots \\ &\quad \overbrace{\qquad\qquad\qquad}^{\text{from } (f(x+h) - f(x-h))/2h} \end{aligned}$$

This hold for any small enough $h > 0$.

$h \leftarrow h/2$ yields

$$f'(x) = \varphi(h/2) - \frac{a_2}{4}h^2 - \frac{a_4}{16}h^4 - \dots$$

$$(\ast\ast) 4f'(x) = 4\varphi(h/2) - a_2 h^2 - \frac{a_4}{4}h^4 - \dots$$

$$\begin{aligned} (\ast\ast) - (\ast) : 3f'(x) &= 4\varphi(h/2) - \varphi(h) + \frac{3}{4}a_4 h^4 + \dots \\ \Rightarrow f'(x) - \underbrace{\frac{1}{3}(4\varphi(h/2) - \varphi(h))}_{=: \psi(h)} &= \frac{3}{4}a_4 h^4 + \dots \end{aligned}$$

where

$$\begin{aligned}\Psi(h) &= \frac{1}{3} (4\varphi(h/2) - \varphi(h)) \\ &= \frac{1}{3} \left(4 \frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{2 \cdot \frac{h}{2}} - \frac{f(x+h) - f(x-h)}{2h} \right) \\ &= \frac{1}{6h} (8f(x+\frac{h}{2}) - 8f(x-\frac{h}{2}) - f(x+h) + f(x-h))\end{aligned}$$

Since $f(x) \approx p(x)$ on $[a, b]$

we expect $\int_a^b f(x) dx \approx \int_a^b p(x) dx$

$$p(x) = \sum_{i=0}^n f(x_i) l_i(x)$$

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

$$\begin{aligned} &= \sum_{i=0}^n f(x_i) \underbrace{\int_a^b l_i(x) dx}_{=: A_i} \\ &= \sum_{i=0}^n f(x_i) A_i \end{aligned}$$

Trapezoidal rule is exact for Π_1

Since Newton-Cotes formula is linear,
it suffices to show that for I, X .

If $f(x) = 1$.

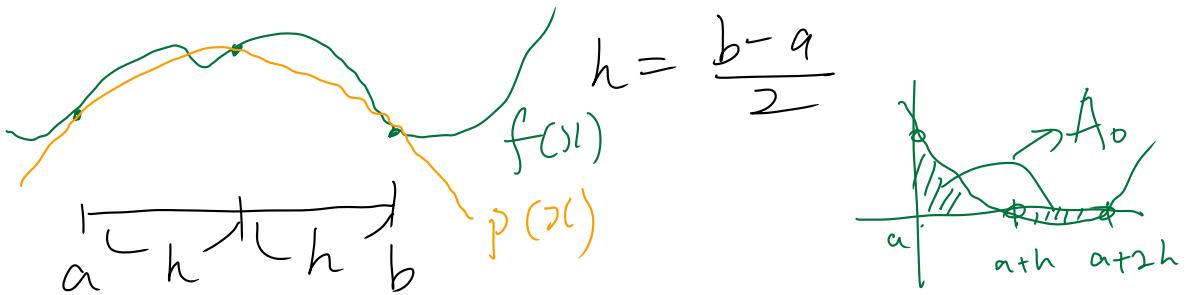
$$\int_a^b 1 dx = b-a$$

$$(b-a) \cdot \frac{f(b)+f(a)}{2} = (b-a) \frac{1+1}{2} = b-a \quad \checkmark$$

If $f(x) = x$

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

$$(b-a) \frac{f(b)+f(a)}{2} = (b-a) \frac{b+a}{2} \quad \checkmark$$



$$A_0 = \int_a^b l_0(x) dx = \int_a^b \frac{(x-a-h)(x-a-2h)}{(x-a-h)(x-a-2h)} dx$$

$$= \int_a^{a+2h} \frac{(x-a-h)(x-a-2h)}{2h^2} dx$$

$$= \frac{1}{2h^2} \int_{-h}^h z(z-h) dz$$

$$z = x - a - h$$

$$dz = dx$$

$$= \frac{1}{2h^2} \int_{-h}^h z^2 - hz dz$$

even

$$= \frac{1}{2h^2} \cdot 2 \left[\frac{z^3}{3} \right]_0^h = \frac{1}{3} h^2$$

$$= \frac{h}{3}$$

Similarly,

$$A_1 = \int_a^{a+2h} \frac{(x-a)(x-a-2h)}{(x+h-a)(x+h-a-2h)} dx$$

$$= -\frac{1}{h^2} \int_{-h}^h (z+h)(z-h) dz$$

$$x - a - h = z$$

$$dx = dz$$

$$\begin{aligned}
 &= -\frac{1}{h^2} \int_{-h}^h z^2 - h^2 dz \\
 &\quad \text{even } \int_0^h z^2 - h^2 dz \\
 &= -\frac{1}{h^2} \cdot 2 \left[\frac{z^3}{3} - h^2 z \right]_0^h \\
 &= \frac{4}{3} h = \frac{h^3}{3} - h^3 = -\frac{2}{3} h^3
 \end{aligned}$$

$$\begin{aligned}
 A_2 &= \int_a^{a+2h} \frac{(x-a)(x-a-h)}{(x+2h-a)(x+2h-a-h)} dx \\
 &= \frac{1}{2h^2} \int_a^{a+2h} (x-a)(x-a-h) dx \quad x-a-h = z \\
 &\quad dx = dz \\
 &= \frac{1}{2h^2} \int_{-h}^h (z+h) z dz \\
 &\quad \text{even } \int_0^h (z+h) z dz \circ (b/c \text{ odd}) \\
 &= \frac{1}{2h^2} \cdot 2 \left[\frac{z^3}{3} \right]_0^h \\
 &= \frac{h}{3}
 \end{aligned}$$

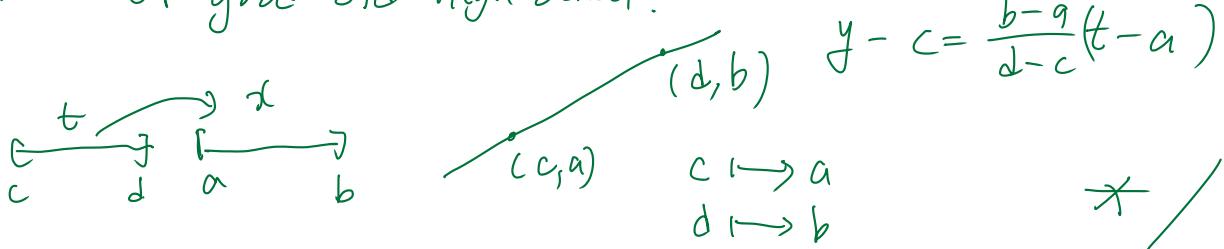
$$\begin{aligned}
 \text{Thus, } \int_a^b f(x) dx &\approx \sum_{i=0}^2 f(x_i) A_i \\
 &= f(a) \frac{h}{3} + f(a+h) \frac{4h}{3} + f(a+2h) \frac{h}{3} \\
 &= \frac{h}{3} (f(a) + 4f(a+h) + f(a+2h)) \\
 &= \frac{b-a}{6} (f(a) + 4f(\frac{b+a}{2}) + f(b))
 \end{aligned}$$

(Quadrature formula for a different interval)

$$\textcircled{1} \text{ find } \lambda(t) \quad \frac{t \mid c \mid d}{x \mid a \mid b}$$

$$\begin{aligned}\text{Lagrange : } \lambda(t) &= a \cdot \frac{t-d}{c-d} + b \cdot \frac{t-c}{d-c} \\ &= \frac{-a}{d-c} t + \frac{ad}{d-c} + \frac{b}{d-c} t - \frac{bc}{d-c} \\ &= \frac{b-a}{d-c} t + \frac{ad-bc}{d-c}\end{aligned}$$

* Or good old High school :



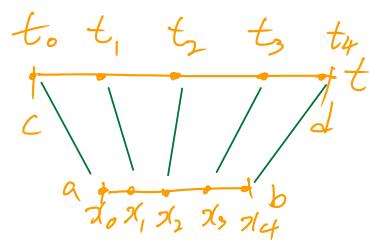
$$\begin{aligned}\textcircled{2} \quad \int_a^b f(x) dx &= \int_c^d f(\lambda(t)) \lambda'(t) dt \\ &\quad \frac{b-a}{d-c} \text{ constant} \\ &\approx \frac{b-a}{d-c} \sum_{i=0}^n f(\lambda(t_i)) \cdot \int_c^d l_i(t) dt\end{aligned}$$

$$\begin{aligned}x &= \lambda(t) \\ dx &= \lambda'(t) dt \\ &= \frac{b-a}{d-c} dt\end{aligned}$$

$$\approx \frac{b-a}{d-c} \sum_{i=0}^n f(\lambda(t_i)) \cdot \int_c^d l_i(t) dt$$

$$= \frac{b-a}{d-c} \sum_{i=0}^n f(\lambda(t_i)) A_i$$

$$\text{where, } t_i = \lambda^{-1}(x_i)$$

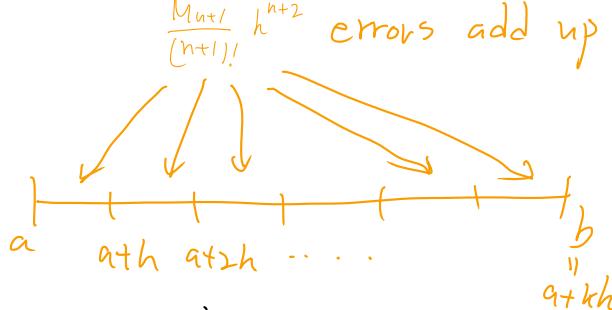


(Error of quadrature)

① Single interval.

$$\begin{aligned}
 & \left| \int_a^{a+h} f(x) - p(x) dx \right| \leq \int_a^{a+h} |f(x) - p(x)| dx \\
 &= \int_a^{a+h} \frac{1}{(n+1)!} \left| f^{(n+1)}(\xi_x) \prod_{i=0}^n (x-x_i) \right| dx \\
 &\leq \frac{1}{(n+1)!} \max_{a \leq x \leq a+h} |f^{(n+1)}(x)| \prod_{i=0}^n |x-x_i| dx \\
 &= \frac{\hat{M}_{n+1}}{(n+1)!} h^{n+1} \int_a^{a+h} dx \\
 &= \frac{\hat{M}_{n+1}}{(n+1)!} h^{n+2}
 \end{aligned}$$

$\hat{M}_{n+1} := \max_{a \leq x \leq a+h} |f^{(n+1)}(x)|$
 $\frac{\hat{M}_{n+1}}{(n+1)!} h^{n+2}$ errors add up.



② Composite rule

$$\begin{aligned}
 & \left| \int_a^b f(x) dx - \sum_{j=1}^k \sum_{i=0}^n f(x_i + (j-1)h) A_i \right| \\
 &= \left| \sum_{j=1}^k \int_{a+(j-1)h}^{a+jh} f(x) dx - \sum_{j=1}^k \sum_{i=0}^n f(x_i + (j-1)h) A_i \right|
 \end{aligned}$$

$$\begin{aligned}
&\leq \sum_{j=1}^k \underbrace{\int_{a+(j-1)h}^{a+jh} \left| f(x) - \sum_{i=0}^n f(x_i + (j-i)h) A_i \right| dx}_{\leq \frac{M_{n+1}}{(n+1)!} h^{n+2}} \\
&\leq \sum_{j=1}^k \frac{M_{n+1}}{(n+1)!} h^{n+2} \quad M_{n+1} := \max_{a \leq x \leq b} |f^{(n+1)}(x)| \\
&= \frac{M_{n+1}}{(n+1)!} h^{n+2} \cdot k \quad (k h = b-a \\
&\quad \text{or } h = \frac{b-a}{k}) \\
&= \frac{M_{n+1}}{(n+1)!} h^{n+1} \cdot (b-a)
\end{aligned}$$

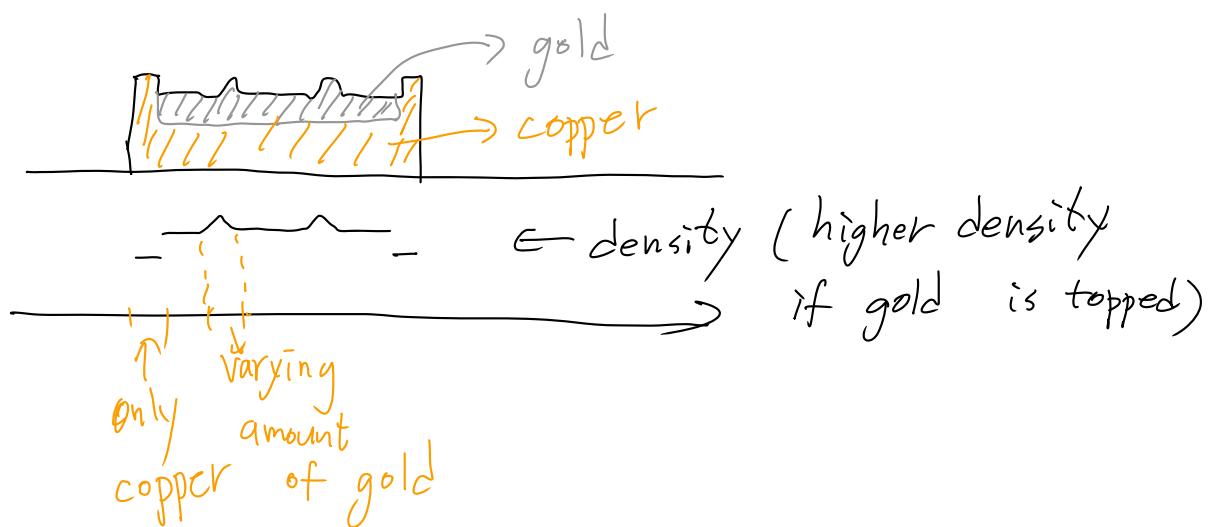
(Example) Error of trapezoidal rule.

$$\left| \int_a^b f(x) dx - \frac{f(b) + f(a)}{2} \cdot (b-a) \right| \leq \frac{\bar{M}_2}{2!} (b-a)^3$$

Composite trapezoidal rule.

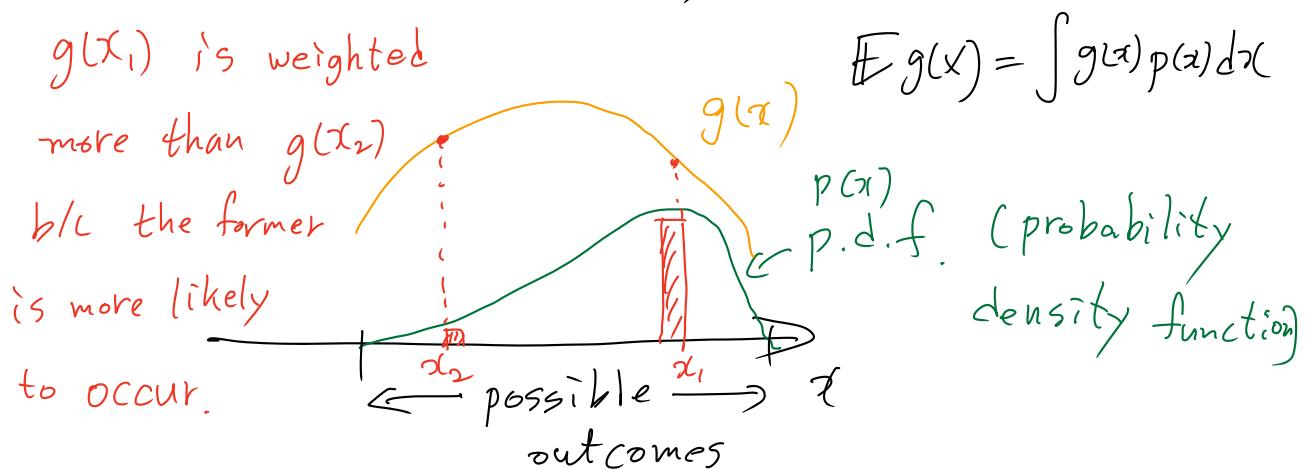
$$\begin{aligned}
&\left| \int_a^b f(x) dx - \frac{h}{2} (f(a) + 2f(a+h) + 2f(a+2h) + \dots + 2f(a+(k-1)h) + f(b)) \right| \\
&\leq \frac{M_2}{2!} h^2 (b-a)
\end{aligned}$$

(Motivation for weighted integral)



$$\begin{aligned} \text{mass} &= \sum \text{area} \cdot \text{density} \\ &= \text{height} \cdot \text{width} \cdot dx \\ &= \int \underbrace{\text{height}}_{f(x)} \cdot \underbrace{\text{density}}_{w(x)} dx \end{aligned}$$

probability : The more likely outcomes are the more they are weighted.



Quadrature rule for weighted integrals

The same idea: $\int_a^b p(x) w(x) dx$ for some

$$p(x) \in \Pi_n \quad \text{s.t.} \quad p(x_i) = f(x_i) \quad i=0, 1, 2, \dots, n$$

$$\begin{aligned} \int_a^b p(x) w(x) dx &= \int_a^b \sum_{i=0}^n l_{x_i}(x) f(x_i) w(x) dx \\ &= \sum_{i=0}^n f(x_i) \underbrace{\int_a^b l_{x_i}(x) w(x) dx}_{\text{call this } \tilde{A}_{x_i}} \\ &= \sum_{i=0}^n f(x_i) \tilde{A}_{x_i} \end{aligned}$$

This formula is Π_n -exact b/c if $f \in \Pi_n$,
 $p(x) = f(x)$ (by uniqueness of interpolating polynomial)

(proof of T_{2n+1} -exactness)

Let $f \in T_{2n+1}$. Then, by division algorithm
there exist $g, r \in T_n$ s.t.

$$f(x) = g(x) \cdot g(x) + r(x)$$

degree degree degree degree
 $\leq 2n+1$ $n+1$ $\leq n$ $\leq n$

$$\begin{aligned}
 \sum_{i=0}^n f(x_i) \tilde{A}_x &= \sum_{i=0}^n (\underbrace{g(x_i) g(x_i)}_{=0} + r(x_i)) \tilde{A}_x && \text{by construction of } g. \\
 &= \sum_{i=0}^n r(x_i) \tilde{A}_x \\
 &= \int_a^b \underbrace{r(x) w(x) dx}_{\in T_n} && \text{(by exactness)} \\
 &= \int_a^b \underbrace{g(x) g(x) w(x) dx}_{=0 \text{ by orthogonality}} + \int_a^b r(x) w(x) dx \\
 &&& \text{of } g \text{ to } T_n \\
 &= \int_a^b (g(x) g(x) + r(x)) w(x) dx \\
 &= \int_a^b f(x) w(x) dx.
 \end{aligned}$$

(example) To find $g \in \Pi_2$ s.t. $g \perp \Pi_1$,
set $g(x) = x^2 + ax + b$ and require ($w(x) \equiv 1$)

$$\underbrace{\int_{-1}^1 g(x) \cdot 1 dx = 0}_{\textcircled{1}} \quad \text{and} \quad \underbrace{\int_{-1}^1 g(x)x dx = 0}_{\textcircled{2}}$$

$$\textcircled{1} \quad \int_{-1}^1 (x^2 + ax + b) dx = 2 \left[\frac{x^3}{3} + bx^2 \right]_0^1 = 2 \cdot \left(\frac{1}{3} + b \right) = 0$$

$$\Rightarrow b = -\frac{1}{3}$$

$$\textcircled{2} \quad \int_{-1}^1 (x^2 + ax - \frac{1}{3})x dx = \int_{-1}^1 x^3 + ax^2 - \frac{1}{3}x^2 dx$$

$$= 2 \left[\frac{ax^3}{3} \right]_0^1 = 2 \cdot \frac{a}{3} = 0$$

$$\Rightarrow a = 0.$$

From ① and ②,

$$g(x) = x^2 - \frac{1}{3} \Rightarrow x_0 = -\frac{1}{\sqrt{3}}, x_1 = \frac{1}{\sqrt{3}}$$

$$\tilde{A}_0 = \int_{-1}^1 \frac{x - \frac{1}{\sqrt{3}}}{-\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}} dx = -\frac{\sqrt{3}}{2} \int_{-1}^1 x - \frac{1}{\sqrt{3}} dx -$$

$$= -\frac{\sqrt{3}}{2} \cdot \left(-\frac{2}{\sqrt{3}} \right) = 1.$$

For \tilde{A}_1 , we use exactness for $f(x) \equiv 1$.

$$\begin{aligned}\int_{-1}^1 dx = 2 &= \tilde{A}_0 f(x_0) + \tilde{A}_1 f(x_1) \\ &= 1 \cdot 1 + \tilde{A}_1 \cdot 1 = 1 + \tilde{A}_1 \\ \Rightarrow \tilde{A}_1 &= 1.\end{aligned}$$

(Example) TI_3 -exactness of $x_0 = -\frac{1}{\sqrt{3}}$
 $x_1 = \frac{1}{\sqrt{3}}$, $A_0 = A_1 = 1$, $w(x) = 1$.

Test $1, x_1, x_1^2, x_1^3$.

(a) $f(x) = 1$ is trivial since we determined A_1 from this condition.

(b) $f(x) = x$

$$(\text{true}) \int_{-1}^1 x dx = 0$$

$$(\text{formula}) A_0 f(x_0) + A_1 f(x_1) = 1 \cdot \left(-\frac{1}{\sqrt{3}}\right) + 1 \cdot \left(\frac{1}{\sqrt{3}}\right) = 0$$

(c) $f(x) = x^2$

$$(\text{true}) \int_{-1}^1 x^2 dx = 2 \left[\frac{x^3}{3} \right]_0^1 = \frac{2}{3}$$

$$(\text{formula}) A_0 f(x_0) + A_1 f(x_1) = 1 \cdot \left(\frac{1}{3}\right) + 1 \cdot \left(\frac{1}{3}\right) = \frac{2}{3}$$

(d) $f(x) = x^3$

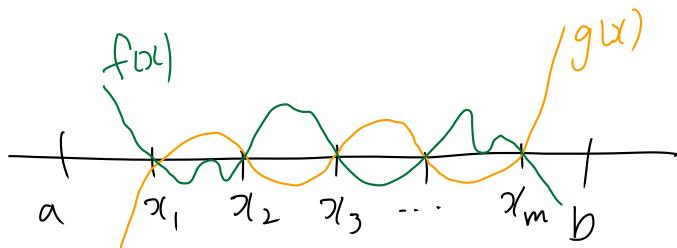
$$(\text{true}) \int_{-1}^1 x^3 dx = 0$$

$$(\text{formula}) A_0 f(x_0) + A_1 f(x_1) = 1 \cdot \left(-\frac{1}{\sqrt{3}^3}\right) + 1 \cdot \left(\frac{1}{\sqrt{3}^3}\right) = 0$$

(proof of thm on sign change)

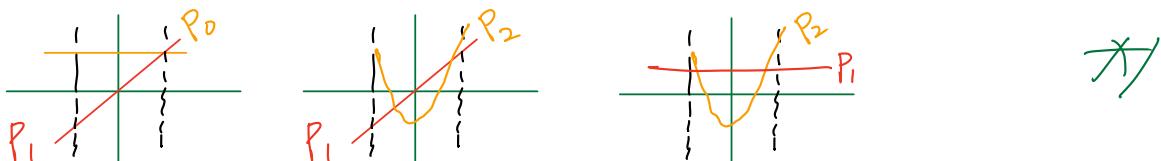
Proof by contradiction. Suppose f changes sign only m times $m \leq n$. Let x_1, x_2, \dots, x_m be where f changes sign : $f(x_j) = 0 \quad j=1, 2, \dots, m$

Let $g(x) = (x-x_1)(x-x_2)\cdots(x-x_m) \in \mathbb{P}_n$. Then, f and g always have either the opposite sign or the same sign. ($g(x) \equiv 1$ if $m=0$ by convention)



Thus, $\int_a^b f(x)g(x)w(x)dx > 0$ or
 $\int_a^b f(x)g(x)w(x)dx < 0$, which contradicts the orthogonality condition.

/* Intuitively speaking orthogonal polynomials get wigglier and wigglier to cancel out the area of their product.



(proof positivity of Gaussian quadrature coeff's)

Gaussian quadrature is exact for

Π_{2n+1} . Since $\underbrace{(\ell_i(x))}_\text{degree } 2n^2 \in \overline{\Pi}_{2n+1}$,

$$0 < \int_a^b (\ell_i(x))^2 w(x) dx = \sum_{j=0}^n \tilde{A}_j \underbrace{(\ell_i(x_j))}_\text{exactness}^2 = \tilde{s}_{ij}$$
$$= \tilde{A}_i$$

Next, Gaussian quadrature is exact
for $f(x) \equiv 1$:

$$\int_a^b 1 \cdot w(x) dx = \sum_{i=0}^n \tilde{A}_i \cdot 1$$

(proof of convergence of Gaussian quadrature)

Given $f \in C[a,b]$, $\exists p(x) \in \Pi_n$ s.t.

$$\|f - p\|_\infty < \varepsilon \quad (\text{Recall } \|g\|_\infty = \max_{a \leq x \leq b} |g(x)|)$$

(We briefly discussed this at the end of approximation theory: Weierstrass Approximation theorem)

Then, we can choose nodes x_0, x_1, \dots, x_m ($2m+1 \geq n$)

s.t. the induced Gaussian quadrature is Π_{2m+1} -exact.

Thus,

$$\pm \int_a^b p(x) w(x) dx$$

$$\left| \int_a^b f(x) w(x) dx - \sum_{i=0}^m \tilde{A}_i f(x_i) \right|$$

$$\leq \left| \int_a^b f(x) w(x) dx - \int_a^b p(x) w(x) dx \right|$$

$$+ \left| \int_a^b p(x) w(x) dx - \sum_{i=0}^m \tilde{A}_i f(x_i) \right|$$

$= \sum_{i=0}^m \tilde{A}_i p(x_i)$ by exactness

$$\leq \int_a^b |f(x) - p(x)| w(x) dx + \sum_{i=0}^m \tilde{A}_i |p(x_i) - f(x_i)|$$

$$\leq \varepsilon \int_a^b w(x) dx + \varepsilon \sum_{i=0}^m \tilde{A}_i$$

$$= 2\varepsilon \underbrace{\int_a^b w(x) dx}_{\text{fixed}}$$

□