(forward/backward diff. quotient)

Taylor:

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

Rearrange:

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

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)

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

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

subtract and rearrange

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

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

Here, we used a little trick.

lemma: Let g is continuous on $[a,b]$.
Then, for any $x_1, x_2, \cdots, x_n \in [a,b]$ there exists $\xi \in [a,b]$ such that

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

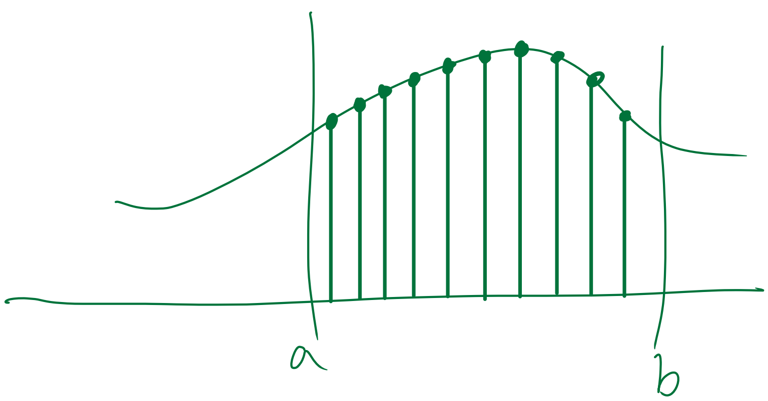
proof) The mean is b/w the maximum and the minimum of g over $[a,b]$. Hence, intermediate value theorem asserts that $\exists \xi$ satisfying $(*)$.

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.

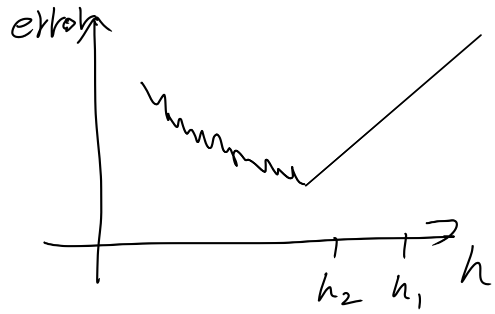


$$\Delta x \approx \frac{b-a}{n} \Rightarrow \frac{1}{n} \approx \frac{\Delta x}{b-a}$$

$$\frac{1}{n}\sum_{i=1}^{n} g(x_i) \approx \frac{1}{b-a}\sum_{i=1}^{n} g(x_i)\Delta x$$

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

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



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

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

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

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

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

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

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

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

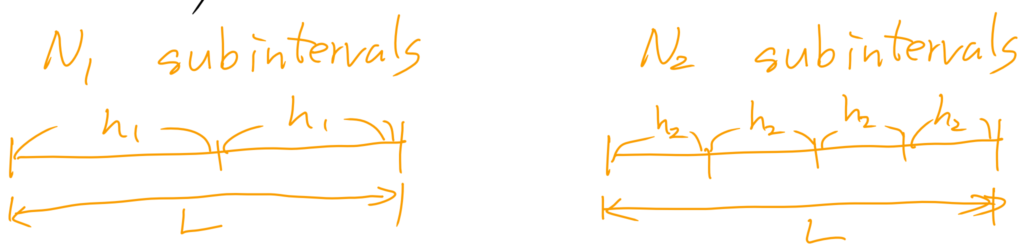
$$e_2 = 2^{-r} e_1 \rightarrow$$

If $r=1$, $e_2 = \frac{1}{2} e_1$
half spacing $\rightarrow$ half error

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.



$h_1 = \frac{L}{N_1}$ $\qquad$ $h_2 = \frac{L}{N_2}$

From the general formula above

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

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2}h^2 + \frac{f'''(x)}{6}h^3 + \frac{f^{(4)}(x)}{24}h^4 + \cdots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2}h^2 - \frac{f'''(x)}{6}h^3 + \frac{f^{(4)}(x)}{24}h^4 + \cdots$$

subtract and rearrange:

$$(*)\quad f'(x) = \varphi(h) - \frac{f'''(x)}{6}h^2 - \frac{f^{(5)}}{5!}h^4 - \cdots$$

$$= \underbrace{\varphi(h)}_{\to\ (f(x+h)-f(x-h))/2h} - a_2h^2 - a_4h^4 - \cdots$$

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

$h \leftarrow h/2$ yields

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

$$(**)\quad 4f'(x) = 4\varphi(h/2) - a_2h^2 - \frac{a_4}{4}h^4 - \cdots$$

$$(**)-(*):\quad 3f'(x) = 4\varphi(h/2) - \varphi(h) + \frac{3}{4}a_4h^4 + \cdots$$

$$\Rightarrow f'(x) - \underbrace{\frac{1}{3}\left(4\varphi(h/2) - \varphi(h)\right)}_{=:\ \psi(h)} = \frac{1}{4}a_4h^4 + \cdots$$

where

$$\psi(h) = \frac{1}{3}\left(4\varphi(h/2) - \varphi(h)\right)$$

$$= \frac{1}{3}\left(4\,\frac{f(x+\frac{h}{2}) - f(x-\frac{h}{2})}{\cancel{2}\cdot\frac{h}{\cancel{2}}} - \frac{f(x+h) - f(x-h)}{2h}\right)$$

$$= \frac{1}{6h}\left(8f(x+\tfrac{h}{2}) - 8f(x-\tfrac{h}{2}) - f(x+h) + f(x-h)\right)$$

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

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

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

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

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

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

Trapezoidal rule is exact for Π_1

Since Newton-Cotes formula is linear, it suffices to show that for $1, x$.

If $f(x) = 1$.

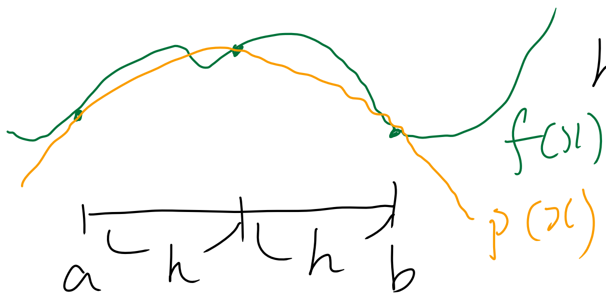
$$\int_a^b 1\,dx = b-a$$

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

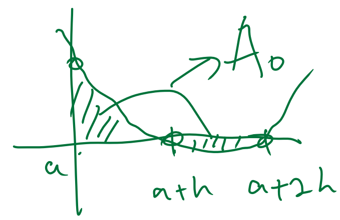
If $f(x) = x$

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

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



$$h = \frac{b-a}{2}$$



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

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

$z = x-a-h$

$dz = dx$

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

$$= \frac{1}{2h^2}\int_{-h}^{h} \underbrace{z^2}_{\text{even}} - \cancel{hz}^{\to 0}\,dz = 2\int_0^h z^2\,dz$$

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

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

Similarly,

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

$x-a-h = z$

$dx = dz$

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

$$= -\frac{1}{h^2}\int_{-h}^{h} \underbrace{z^2 - h^2}_{\text{even}}\, dz \quad = 2\int_0^h z^2 - h^2\, dz$$

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

$$= \frac{4}{3}h$$

$$A_2 = \int_a^{a+2h} \frac{(x-a)(x-a-h)}{(\cancel{a}+2h-\cancel{a})(\cancel{a}+2h-\cancel{a}-h)}\, dx$$

$$= \frac{1}{2h^2}\int_a^{a+2h} (x-a)(x-a-h)\, dx \qquad x-a-h = z, \quad dx = dz$$

$$= \frac{1}{2h^2}\int_{-h}^{h} \underbrace{(z+h)z}_{\text{even } z^2 + \cancel{hz} \to 0 \text{ (b/c odd)}}\, dx$$

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

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

Thus, $\int_a^b f(x)\,dx \approx \sum_{i=0}^{2} f(x_i)A_i$

$$= f(a)\frac{h}{3} + f(a+h)\frac{4h}{3} + f(a+2h)\frac{h}{3}$$

$$= \frac{h}{3}\left(f(a) + 4f(a+h) + f(a+2h)\right)$$

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

(Quadrature formula for a different interval)

① find $\lambda(t)$

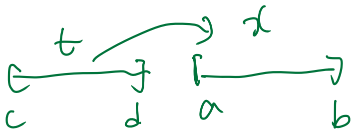
t	c	d
x	a	b

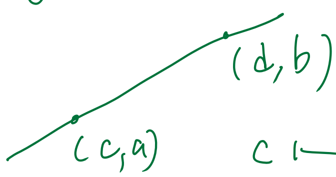
Lagrange : $\lambda(t) = a \cdot \dfrac{t-d}{c-d} + b\,\dfrac{t-c}{d-c}$

$$= \frac{-a}{d-c}t + \frac{ad}{d-c} + \frac{b}{d-c}t - \frac{bc}{d-c}$$

$$= \frac{b-a}{d-c}t + \frac{ad-bc}{d-c}$$

/* Or good old High School :





$y - c = \dfrac{b-a}{d-c}(t-a)$

$c \longmapsto a$

$d \longmapsto b$

*/

② $\displaystyle\int_a^b f(x)\,dx = \int_c^d f(\lambda(t))\,\underbrace{\lambda'(t)}_{\text{constant}}\,dt$

$\dfrac{b-a}{d-c}$

$x = \lambda(t)$

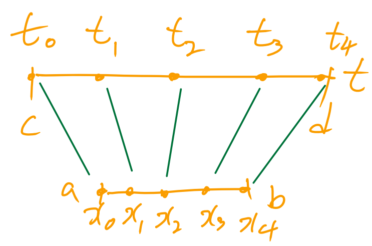
$dx = \lambda'(t)\,dt$

$= \dfrac{b-a}{d-c}\,dt$

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

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

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



(Error of quadrature)

① Single interval.

$$\left|\int_a^{a+h} f(x) - p(x)\,dx\right| \le \int_a^{a+h} |f(x) - p(x)|\,dx$$

$$= \int_a^{a+h} \frac{1}{(n+1)!}\left| f^{(n+1)}(\xi_x) \prod_{i=0}^{n} (x - x_i)\right| dx$$

$$\le \frac{1}{(n+1)!} \max_{a \le x \le a+h} |f^{(n+1)}(x)| \prod_{i=0}^{n} \underbrace{|x - x_i|}_{\le h}\, dx$$

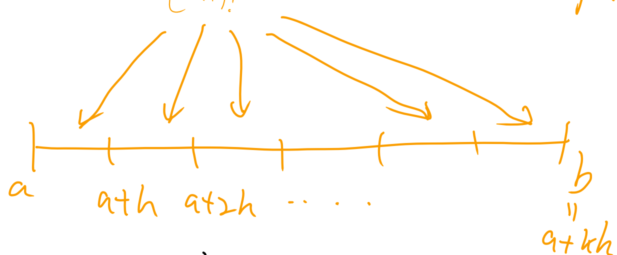
$$= \frac{\hat{M}_{n+1}}{(n+1)!} h^{n+1} \int_a^{a+h} dx$$

$$\hat{M}_{n+1} := \max_{a \le x \le a+h} |f^{(n+1)}(x)|$$

$$= \frac{\hat{M}_{n+1}}{(n+1)!} h^{n+2}$$

$\frac{\hat{M}_{n+1}}{(n+1)!} h^{n+2}$ errors add up.

② Composite rule



$$\left| \int_a^b f(x)\,dx - \sum_{j=1}^{k} \sum_{i=0}^{n} f(x_i + (j-1)h) A_i \right|$$

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

$$\le \sum_{j=1}^{k} \underbrace{\int_{a+(j-1)h}^{a+jh} \left| f(x) - \sum_{i=0}^{n} f(x_i+(j-1)h)A_i \right|}_{\le \frac{\hat{M}_{n+1}}{(n+1)!} h^{n+2}}$$

$$\le \sum_{j=1}^{k} \frac{M_{n+1}}{(n+1)!} h^{n+2} \qquad M_{n+1} := \max_{a \le x \le b} \left| f^{(n+1)}(x) \right|$$

$$= \frac{M_{n+1}}{(n+1)!} h^{n+2} \cdot k \qquad \left(kh = b-a \quad b/c \quad h = \frac{b-a}{k} \right)$$

$$= \frac{M_{n+1}}{(n+1)!} h^{n+1} \cdot (b-a)$$

(Example) Error of trapezoidal rule.

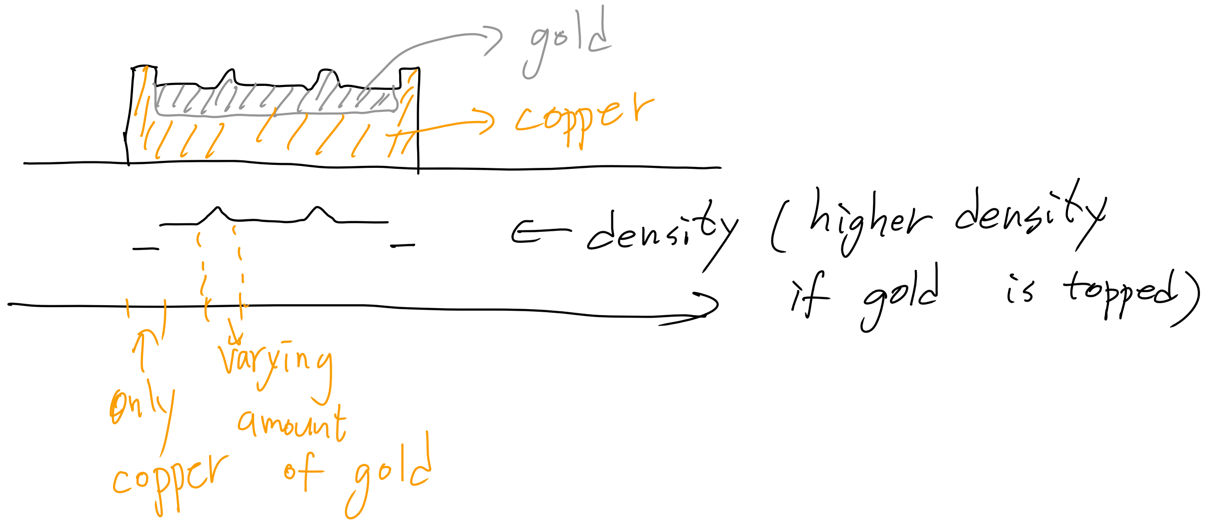
$$\left| \int_a^b f(x)\,dx - \frac{f(b)+f(a)}{2} \cdot (b-a) \right| \le \frac{\hat{M}_2}{2!} (b-a)^3$$

Composite trapezoidal rule.

$$\left| \int_a^b f(x)\,dx - \frac{h}{2} \left(f(a) + 2f(a+h) + 2f(a+2h) + \cdots + 2f(a+(k-1)h) + f(b) \right) \right|$$

$$\le \frac{M_2}{2!} h^2 (b-a)$$

(Motivation for weighted integral)



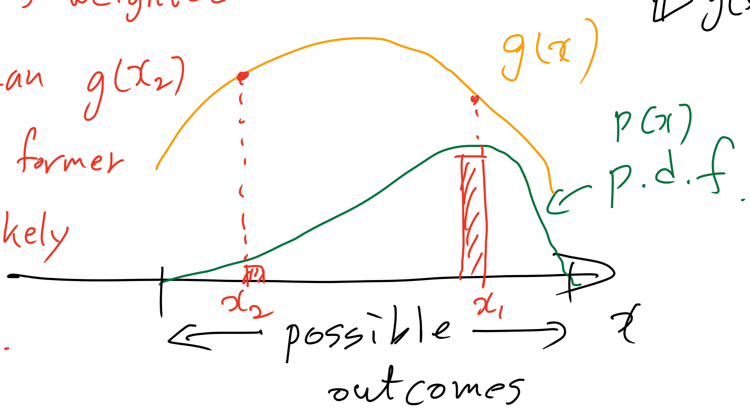
$$\text{mass} = \sum \underbrace{\text{area}}_{= \text{height} \cdot \underbrace{\text{width}}_{\to dx}} \cdot \text{density}$$

$$= \int \underbrace{\text{height}}_{f(x)} \cdot \underbrace{\text{density}}_{w(x)} \, dx$$

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

$g(x_1)$ is weighted more than $g(x_2)$ b/c the former is more likely to occur.

$$\mathbb{E}\, g(X) = \int g(x) p(x) \, dx$$



(probability density function)

Quadrature rule for weighted integrals

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

$p(x) \in \Pi_n$ s.t. $p(x_i) = f(x_i)$ $i = 0, 1, 2, \cdots, n$

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

$$= \sum_{i=0}^{n} f(x_i) \underbrace{\int_a^b l_i(x)\,w(x)\,dx}_{\text{call this } \breve{A}_i}$$

$$= \sum_{i=0}^{n} f(x_i)\,\breve{A}_i$$

This formula is Π_n-exact b/c if $f \in \Pi_n$, $p(x) = f(x)$ (by uniqueness of interpolating polynomial) (proof of Π_{2n+1}-exactness)

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

$$\underbrace{f(x)}_{\substack{\text{degree} \\ \leq 2n+1}} = \underbrace{q(x)}_{\substack{\text{degree} \\ n+1}} \cdot \underbrace{g(x)}_{\substack{\text{degree} \\ \leq n}} + \underbrace{r(x)}_{\substack{\text{degree} \\ \leq n}}$$

$$\sum_{i=0}^{n} f(x_i)\tilde{A}_i = \sum_{i=0}^{n} (\underbrace{q(x_i)}_{=0}g(x_i) + r(x_i))\tilde{A}_i$$

$=0$. by construction of q.

$$= \sum_{i=0}^{n} r(x_i)\tilde{A}_i$$

$$= \int_a^b \underbrace{r(x)}_{\in \Pi_n} w(x)\,dx \quad (\text{by exactness})$$

$$= \underbrace{\int_a^b q(x)g(x)w(x)\,dx}_{=0} + \int_a^b r(x)w(x)\,dx$$

$=0$ by orthogonality of q to Π_n

$$= \int_a^b (q(x)g(x) + r(x))w(x)\,dx$$

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

(example) To find $q \in \Pi_2$ s.t. $q \perp \Pi_1$,

set $q(x) = x^2 + ax + b$ and require $(w(x) \equiv 1)$

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

① $\displaystyle\int_{-1}^{1} \underbrace{x^2 + \cancel{ax}^{\,0\ (\text{odd})} + b}_{\text{even}} \, dx = 2\left[\frac{x^3}{3} + bx\right]_0^1 = 2 \cdot \left(\frac{1}{3} + b\right) = 0$

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

② $\displaystyle\int_{-1}^{1} \left(x^2 + ax - \frac{1}{3}\right) x \, dx = \int_{-1}^{1} \cancel{x^3}^{\,0\ (\text{odd})} + ax^2 - \cancel{\frac{1}{3}x}^{\,0\ (\text{odd})} \, dx$

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

$$\Rightarrow \quad a = 0.$$

From ① and ②,

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

$$\tilde{A}_0 = \int_{-1}^{1} \frac{x - \frac{1}{\sqrt{3}}}{-\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}} \, dx = -\frac{\sqrt{3}}{2} \int_{-1}^{1} \cancel{x}^{\,0\ (\text{odd})} - \frac{1}{\sqrt{3}} \, dx$$

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

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

$$\int_{-1}^{1} dx = 2 = \breve{A}_0 f(x_0) + \breve{A}_1 f(x_1)$$

$$= 1 \cdot 1 + \breve{A}_1 \cdot 1 = 1 + \breve{A}_1$$

$$\Rightarrow \breve{A}_1 = 1.$$

(Example) Π_3-exactness of $x_0 = -\frac{1}{\sqrt{3}}$

$x_1 = \frac{1}{\sqrt{3}}$, $\tilde{A}_0 = \tilde{A}_1 = 1$, $w(x) = 1$.

Test $1, x, x, x^3$.

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

(b) $f(x) = x$

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

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

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

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

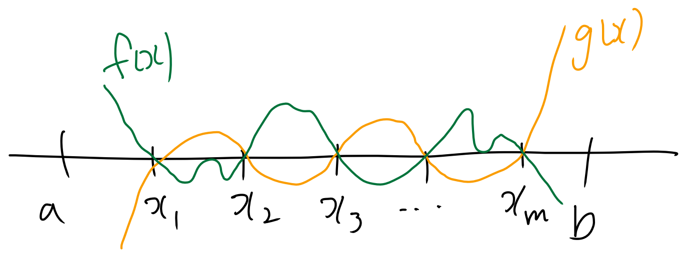
(true) $\int_{-1}^{1} x^3 \, dx = 0$

(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)

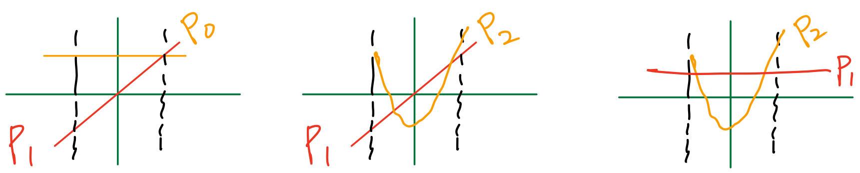
Proof by contradiction. Suppose f changes sign only m times $m \leq n$. Let $x_1, x_2, \cdots, x_m$ be where f changes sign: $f(x_j) = 0$ $j = 1, 2, \cdots, m$

Let $g(x) = (x - x_1)(x - x_2)\cdots(x - x_m) \in \Pi_n$. Then, f ang 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 $\big(\underbrace{\ell_i(x)}_{\text{degree } 2n}\big)^2 \in \Pi_{2n+1}$,

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

$$= \tilde{A}_i$$

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.

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

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

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

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

Thus,

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

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

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

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

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

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

$\boxtimes$