NA Slides
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(based on
Numerical Mathematics and
Computing—Cheney/Kincaid)

Numerical Quadrature

- $\Rightarrow$ Introduction
- Riemann Integration
- Composite Trapezoid Rule
- Composite Simpson's Rule
- Guassian Quadrature

Numerical Quadrature—Motivation

- Analytical solutions—rare:

$$\int_0^{\frac{\pi}{2}} \sin x \, dx = -\cos x|_0^{\frac{\pi}{2}} = -(0-1) = 1$$

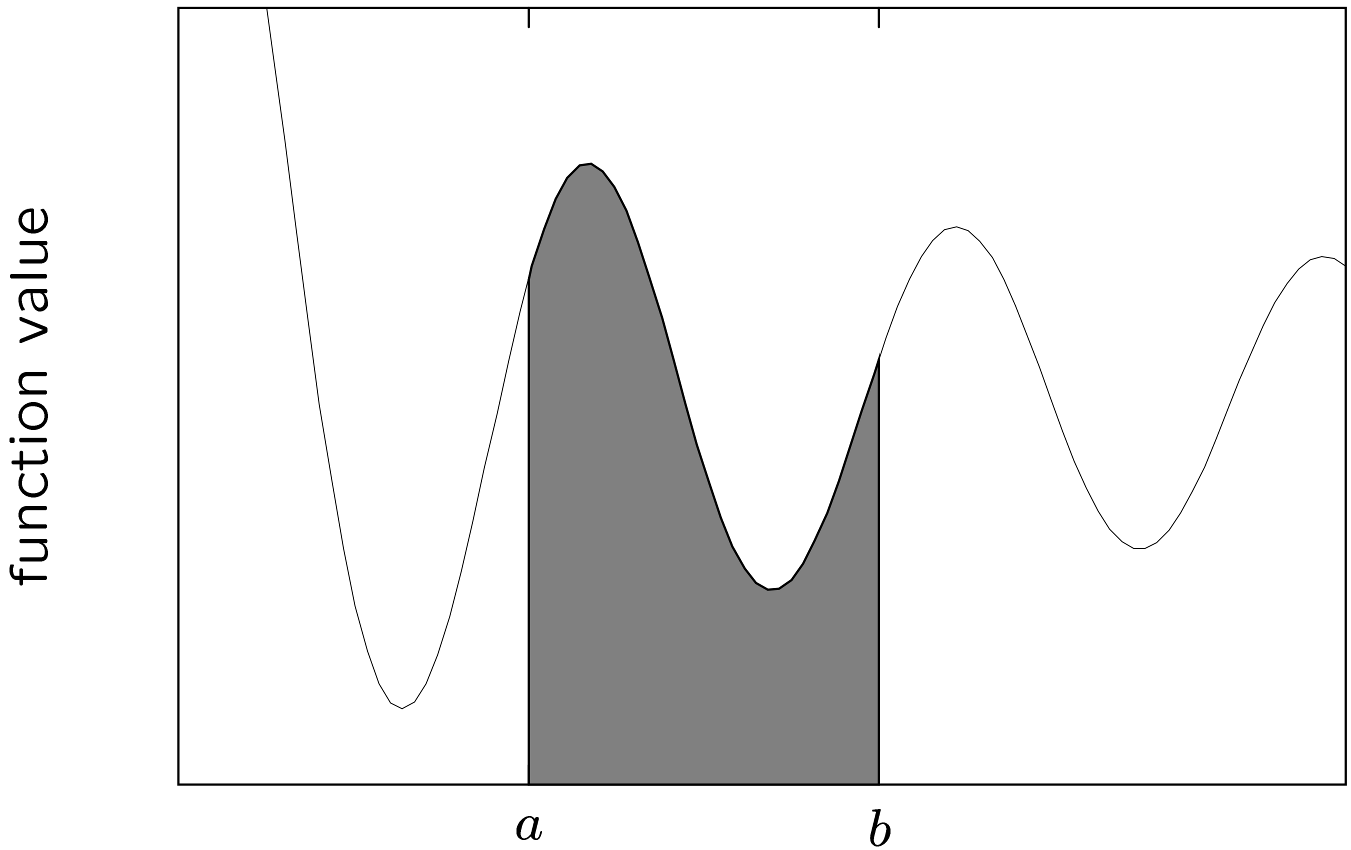
- In general:

$$\int_0^{\frac{\pi}{2}} \left[1 - a^2 \sin^2 \theta\right]^{\frac{1}{3}} d\theta$$

$$\boxed{\text{Need general numerical technique.}}$$

Numerical Quadrature—Interpretation

- $f(x) \geq 0$ on $[a, b]$ bounded $\Rightarrow \int_a^b f(x)\,dx$ is area under $f(x)$



Definitions

- Mesh: $P \equiv \{a = x_0 < x_1 < \cdots < x_n = b\}$, n intervals ($n + 1$ points)

- Infima and suprema:

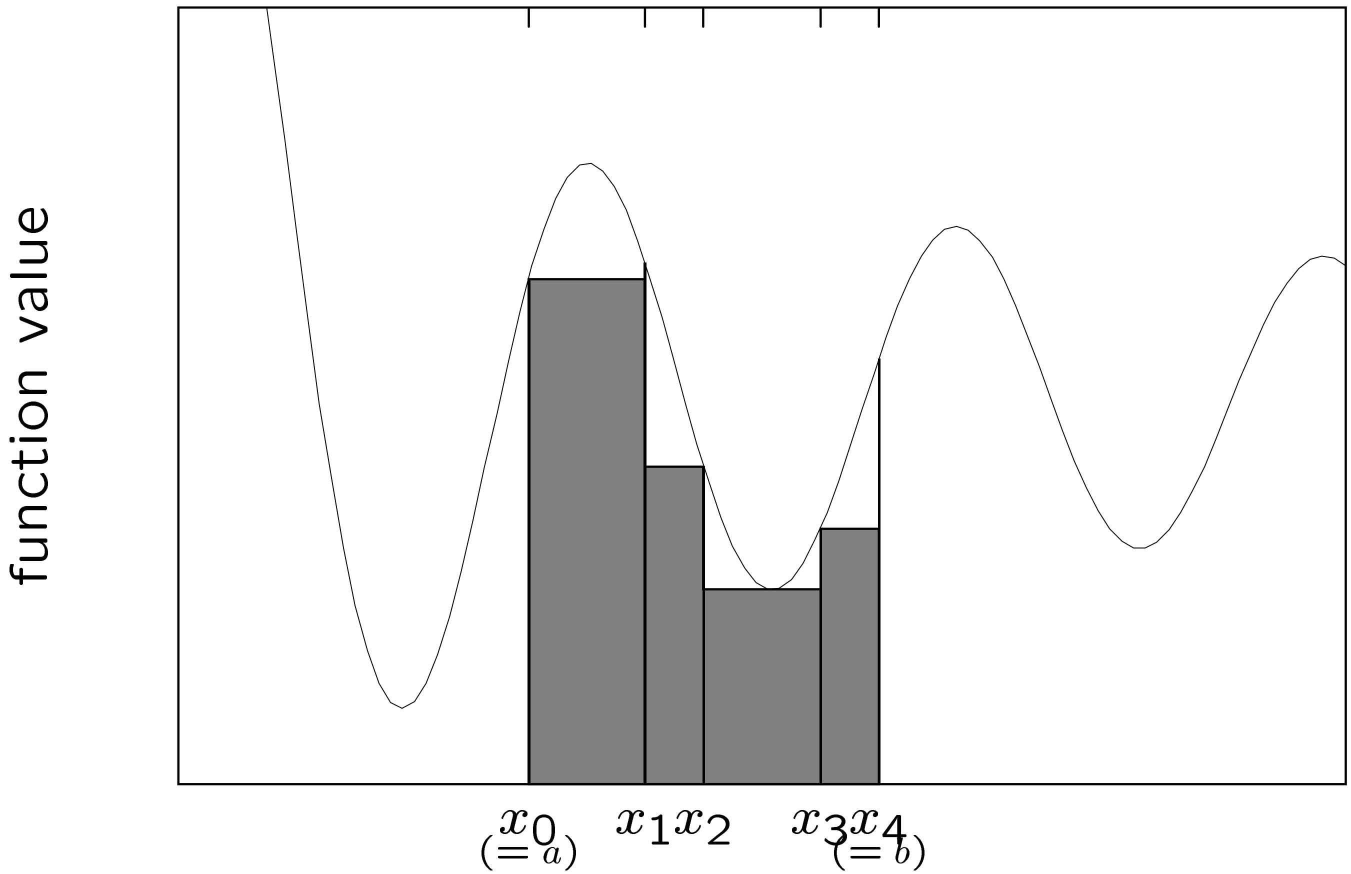
$$
\begin{aligned}
m_i &\equiv \inf \Big\{ f(x) : x_i \le x \le x_{i+1} \Big\} \\
M_i &\equiv \sup \Big\{ f(x) : x_i \le x \le x_{i+1} \Big\}
\end{aligned}
$$

- Lower and upper sums:

$$
\begin{aligned}
L(f; P) &\equiv \sum_{i=0}^{n-1} m_i \Big(x_{i+1} - x_i \Big) \\
U(f; P) &\equiv \sum_{i=0}^{n-1} M_i \Big(x_{i+1} - x_i \Big)
\end{aligned}
$$

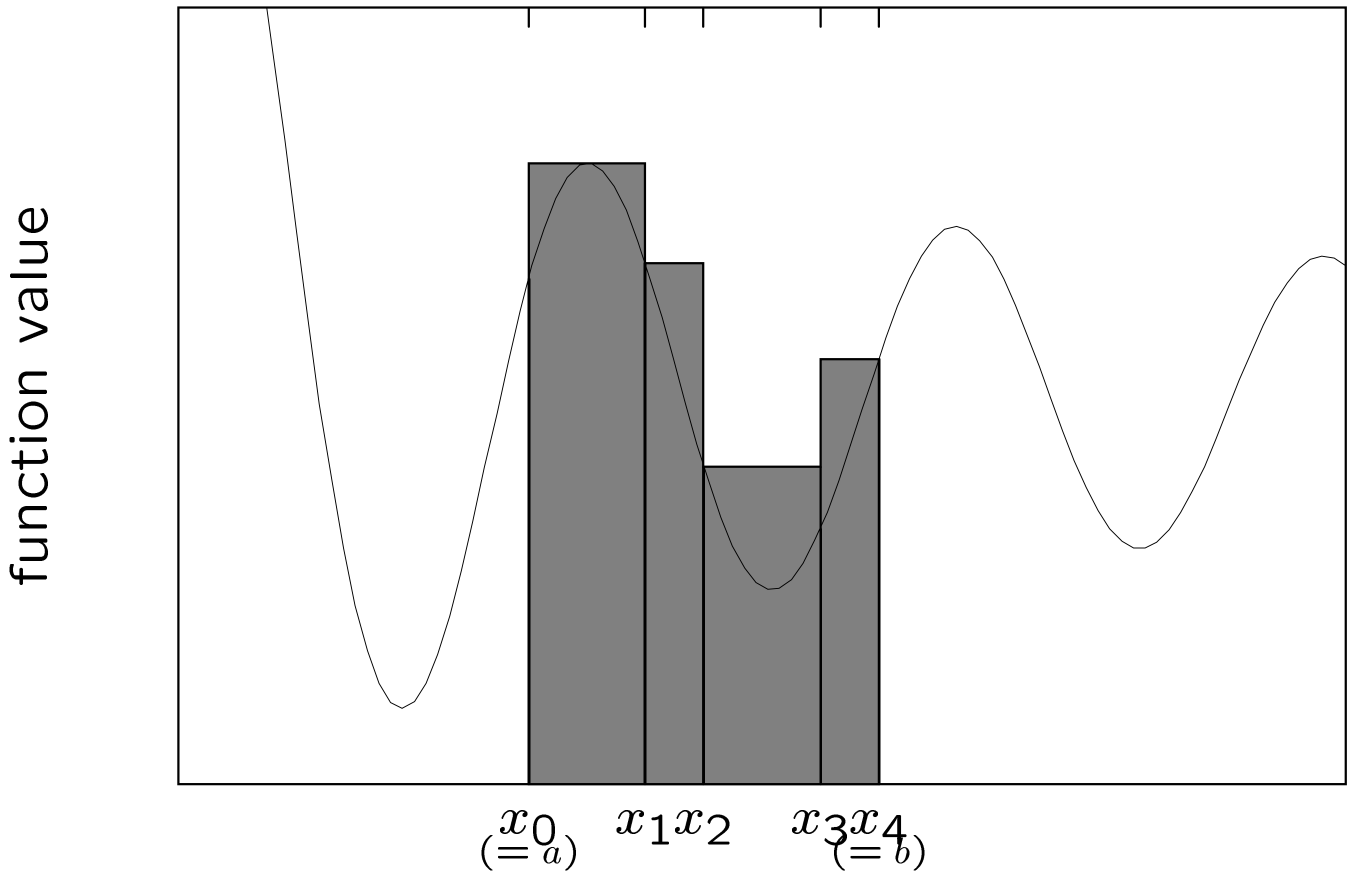
- For example, ...

Lower Sum—Interpretation



Clearly a lower bound of integral estimate, and ...

Upper Sum—Interpretation



. . . an upper bound. What is the error?

Lower and Upper Sums—Example

- $f(x) = x^2$, $[a, b] = [0, 1]$ and $P = \left\{0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1\right\}$
- $\ldots$, $L = \frac{7}{32}$, $U = \frac{15}{32}$
- Split the difference: estimate $\frac{11}{32}$ (actual $\frac{1}{3}$)

Naive approach and low n, still error of $\frac{1}{96}$. (!)

Numerical Quadrature—Rethinking

- Perhaps lower and upper sums are enough?
    - $*$ Error seems small
    - $*$ Work seems small as well

- Do they converge to integral as $n \to \infty$?

$\boxed{\text{Proceed in theoretical and practical directions.}}$

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$\Rightarrow$ Riemann Integration

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Riemann Integrability

- $f \in C^0([a,b])$, $[a,b]$ bdd $\Rightarrow f$ is Riemann integrable
- Counter example: Dirichlet function $d(x) \equiv \begin{cases} 0, & x \text{ rational,} \\ 1, & x \text{ irrational} \end{cases}$

  $\Rightarrow L = 0, \;\; U = b - a$
- When integrable, and max interval in $P \to 0$:

$$\lim_{n\to\infty} L(f;P) = \int_a^b f(x)\,dx = \lim_{n\to\infty} U(f;P)$$

Challenge: Estimate n

- Restrictions for example:
  - $*$ Monotone functions
  - $*$ Uniform partition
- Challenge:
  - $*$ $\int_0^{\pi} e^{\cos x}\,dx$
  - $*$ error $< \frac{1}{2} \times 10^{-3}$
  - $*$ using L and U
  - $*$ $n =$?

Estimate n—Solution

- $f(x) = e^{\cos x} \searrow$ on $[0, pi]$ $\therefore m_i = f\left(x_{i+1}\right)$ and $M_i = f(x_i)$
- $\therefore L(f;P) = h \sum_{i=0}^{n-1} f\left(x_{i+1}\right)$ and $U(f;P) = h \sum_{i=0}^{n-1} f(x_i)$
- Want $\frac{1}{2}(U - L) < \frac{1}{2} \times 10^{-3}$ or $\frac{\pi}{n}\left(e^1 - e^{-1}\right) < \times 10^{-3}$
- $\ldots\ n \geq 7385$ (!!)
- Note: 2 $f(x)$ evaluations for $(U - L)$, but > 7000 for either one

$\boxed{\text{We need something better.}}$

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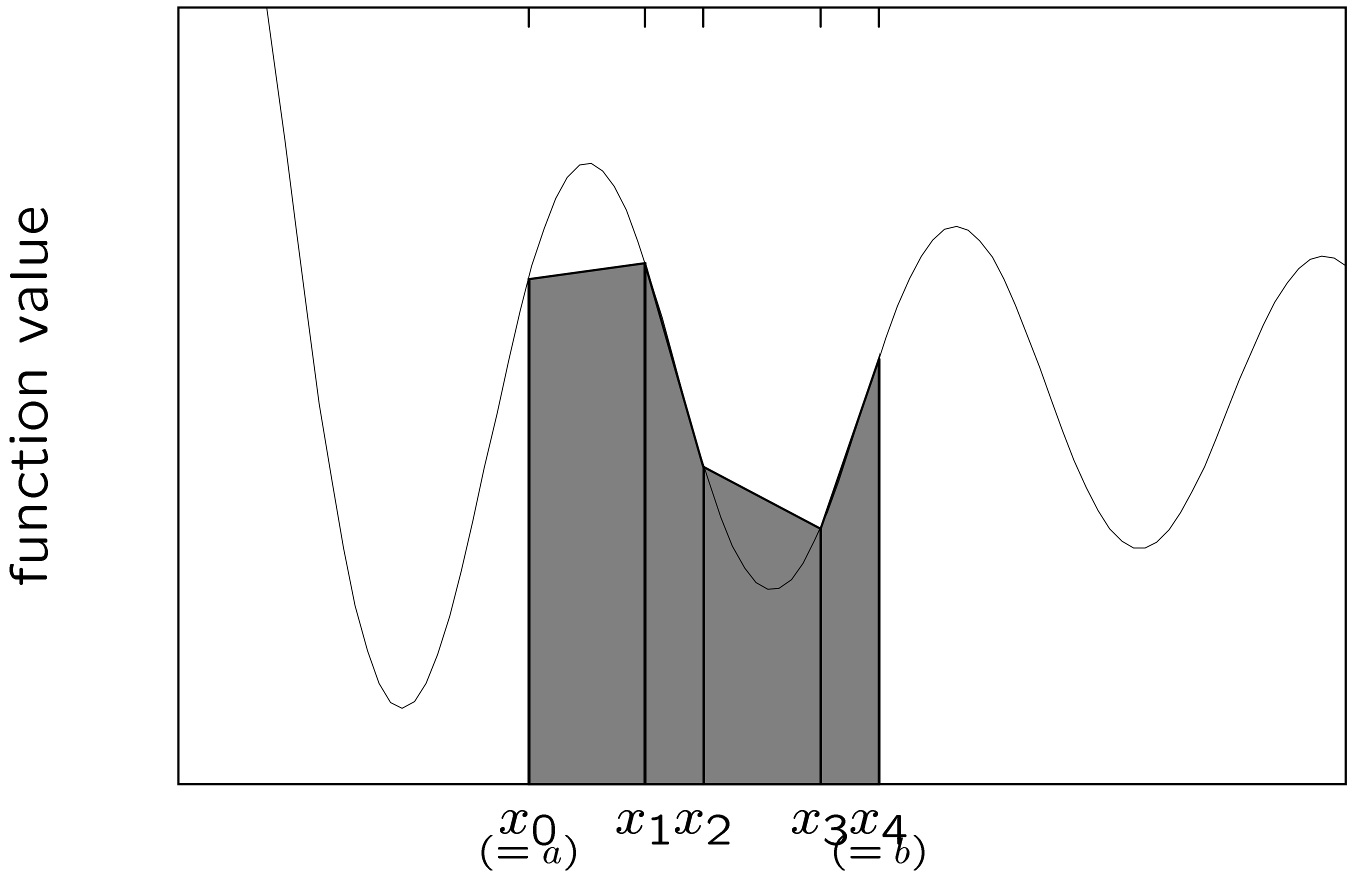
Composite Trapezoid Rule (CTR)

- Each area: $\frac{1}{2}\Big(x_{i+1} - x_i\Big)\Big[f(x_i) + f\Big(x_{i+1}\Big)\Big]$
- Rule: $T(f;P) \equiv \frac{1}{2}\sum_{i=0}^{n-1}\Big(x_{i+1} - x_i\Big)\Big[f(x_i) + f\Big(x_{i+1}\Big)\Big]$
- Note: for monotone functions (any mesh): $T = (U + L)/2$

$\boxed{\text{What does this look like?}}$

CTR—Interpretation



Almost always better than L or U. (When not?)

Uniform Mesh and Error

- Constant stepsize h

$$T(f;P) \equiv h\left\{\sum_{i=0}^{n-1} f(x_i) + \frac{1}{2}[f(x_0) + f(x_n)]\right\}$$

- Theorem: $f \in C^2([a,b]) \to \exists \xi \in (a,b) \ni$

$$\int_a^b f(x)\,dx - T(f;P) = -\frac{1}{12}(b-a)h^2 f''(\xi) = O\big(h^2\big)$$

- Note: leads to Romberg algorithm (built on Richardson extrapolation)

$\boxed{\text{How many steps does } T(f;P) \text{ require?}}$

$e^{\cos x}$ Revisited

- Challenge: $\int_0^{\pi} e^{\cos x}\,dx$, error $< \frac{1}{2} \times 10^{-3}$, using T, $n = ?$

- $f(x) = e^{\cos x} \Rightarrow f'(x) = -e^{\cos x}\sin x \ \ldots\ |f''(x)| \leq e$ on $[0, \pi]$

- $\therefore$ $|\text{error}| < \frac{1}{12}\pi(\pi/n)^2 e < \frac{1}{2} \times 10^{-3}$

- $\ldots\ n \geq 119$

- Recall: monotonic $\therefore$ identical to $(L + U)/2$, *but* L and U used loose error bounds

$$\boxed{\text{Better estimate of } \textit{error} \therefore \text{ better estimate of } n}$$

Another CTR Example

- Challenge: $\int_0^1 e^{-x^2}\,dx$, error $< \frac{1}{2} \times 10^{-4}$, $n = ?$
- $f(x) = e^{-x^2}$, $\Rightarrow$ $f'(x) = -2xe^{-x^2}$ and $f''(x) = \Big(4x^2 - 2\Big)e^{-x^2}$
- $\therefore \left|f''(x)\right| \le 2$ on $[0, 1]$
- $\Rightarrow$ $|\text{error}| \le \frac{1}{6}h^2 \le \frac{1}{2} \times 10^{-4}$
- We have: $n^2 \ge \frac{1}{3} \times 10^4$ or $n \ge 58$ subintervals

$\boxed{\text{How can we do better?}}$

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CTR on Two Intervals

- $n = 2$ (i.e., 3 points):

$$\begin{aligned} T(f) &= \frac{b-a}{2}\left\{f\left(\frac{a+b}{2}\right) + \frac{1}{2}[f(a) + f(b)]\right\} \\ &= \frac{b-a}{4}\left[f(a) + 2f\left(\frac{a+b}{2}\right) + f(b)\right] \end{aligned}$$

  with error $= O\left(\left(\frac{b-a}{2}\right)^2\right)$

- Note: trapezoid rule is integral of linear interpolant on each interval

$$p_1(x) = \frac{x-b}{a-b}f(a) + \frac{x-a}{b-a}f(b)$$

- $\int_a^b p_1(x)\,dx$ calculation ...

Trapezoid Rule as $\int$Interpolant

(Note: this is intuitive.)

$$
\begin{aligned}
\int_a^b p_1(x)\,dx &= \frac{f(a)}{a-b}\int_a^b (x-b)\,dx + \frac{f(b)}{b-a}\int_a^b (x-a)\,dx \\
&= \frac{f(a)}{a-b}\left[\frac{b^2-a^2}{2} - b(b-a)\right] + \frac{f(b)}{b-a}\left[\frac{b^2-a^2}{2} - a(b-a)\right] \\
&= -f(a)\left[\frac{a+b}{2} - b\right] + f(b)\left[\frac{a+b}{2} - a\right] \\
&= -f(a)\left(\frac{a-b}{2}\right) + f(b)\left(\frac{b-a}{2}\right) \\
&= \frac{b-a}{2}(f(a)+f(b))
\end{aligned}
$$

$\boxed{\text{CTR is integral of composite linear interpolant.}}$

Simpson's Rule Over Two Intervals

- Motivation: use $p_2(x)$ over the two intervals
- Similar analysis actually loses $O(h)$, but ... $\exists \xi \in (a,b) \ni$

$$\int_a^b f(x)\,dx = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\xi)$$

- Similar to CTR, but weights midpoint more
- Note: for each method, denominator $= \sum$ coefficients

$\boxed{\text{Each method multiplies width by weighted average of height.}}$

Composite Simpson's Rule (CSR)

- For n even intervals, $h = \frac{b-a}{n}$, $\exists \xi \in (a,b) \ni$

$$\int_a^b f(x)\,dx = \frac{h}{3}\Bigg\{[f(a)+f(b)] + 4\sum_{i=1}^{n/2} \underbrace{f[a+(2i-1)h]}_{\text{interval midpoints}} + 2\sum_{i=1}^{(n-2)/2} \underbrace{f(a+2ih)}_{\text{internal interval boundaries}}\Bigg\} - \frac{b-a}{180}h^4 f^{(4)}(\xi)$$

- Note: denominator $= \sum$ coefficients $= 3n$
(but $2n+1$ function evaluations)

- Another accuracy angle: error $= 0\ \forall f \in P_3$

$$\boxed{\text{Can we do better than } P_3\text{?}}$$

Integration Introspection

- Simpson beat CTR (for $n = 2$) because heavier weighted midpoint

- But CSR similarly suffers at interval boundaries (weight $= 2$ vs. 4)

- All composite rules
  - patch together local calculations
  - $\therefore$ will suffer from this

- What about higher degree interpolation?

- Also: we are choosing
  - calculation nodes
  - weights

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$\Rightarrow$ Guassian Quadrature

Interpolatory Quadrature

- $x_i, \ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \dfrac{x - x_j}{x_i - x_j}, \; i = 0, \cdots, n, \; p(x) = \sum_{i=0}^{n} f(x_i)\ell_i(x)$
- If $f(x) \approx p(x) \Rightarrow$ hopefully $\int_a^b f(x)\,dx \approx \int_a^b p(x)\,dx$
- $\int_a^b p(x)\,dx = \int_a^b \sum_{i=0}^{n} f(x_i)\ell_i(x)\,dx = \sum_{i=0}^{n} f(x_i) \underbrace{\int_a^b \ell_i(x)\,dx}_{\equiv A_i}$
- $A_i = A_i\Big(a, b; \{x_j\}_{j=0}^{n}\Big)$, but $A_i \neq A_i(f)$!

$$\boxed{\text{(Endpoints, nodes)} \Rightarrow A_i \Rightarrow \int_a^b f(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i).}$$

Interp. Quad.—Error Analysis

- $\forall f \in P_n \Rightarrow f(x) = p(x)$, and $\therefore$

  $$\forall f \in P_n \Rightarrow \int_a^b f(x)\,dx = \sum_{i=0}^{n} A_i f(x_i), \text{ i.e., error} = 0$$

- $n+1$ weights determined by nodes x_i (and a and b)
- True for *any* choice of $n+1$ nodes x_i
- What if we choose $n+1$ *specific* nodes (with weights, total: $2(n+1)$ choices)?

$$\boxed{\text{Can we get error} = 0\ \forall f \in P_{2n+1}?}$$

Gaussian Quadrature (GQ)—Theorem

- Let
  - $q(x) \in P_{n+1} \ni \int_a^b x^k q(x)\,dx = 0, \;\; k = 0, \cdots, n$
    i.e., $q(x) \perp$ all polynomials of lower degree
  - $x_i, i = 0, \cdots, n, \ni q(x_i) = 0$
    i.e., x_i are zeros of $q(x)$

- Then $\forall f \in P_{2n+1}$

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

$$\boxed{\text{We jumped from } P_n \text{ to } P_{2n+1}!}$$

Gaussian Quadrature—Proof

- Let $f \in P_{2n+1}$, and divide by $q \ni f = pq + r \therefore p, r \in P_n$
- We have

$$
\begin{aligned}
\int_a^b f(x)\,dx &= \int_a^b p(x)q(x)\,dx + \int_a^b r(x)\,dx && \text{(division above)} \\
&= \int_a^b r(x)\,dx && (\perp'\text{ity of } q(x)) \\
&= \sum_{i=0}^n A_i r(x_i) && (r \in P_n) \\
&= \sum_{i=0}^n A_i [f(x_i) - p(x_i)q(x_i)] && \text{(division above)} \\
&= \sum_{i=0}^n A_i f(x_i) && (x_i \text{ are zeros of } q(x))
\end{aligned}
$$

■

GQ—Additional Notes

- Example $q_n(x)$: Legendre Polynomials: for $[a,b]=[-1,1]$ and $q_n(1)=1$ ($\exists$ a 3-term recurrence formula)

$$q_0(x)=1,\ \ q_1(x)=x,\ \ q_2(x)=\frac{3}{2}x^2-\frac{1}{2},\ \ q_3(x)=\frac{5}{2}x^3-\frac{3}{2}x,\cdots$$

- Gaussian nodes $\in (a,b) \Rightarrow$

  good if $f(a)=\infty$ and/or $f(b)=\infty$ (e.g., $\displaystyle\int_0^1 \frac{1}{\sqrt{x}}\,dx$)

- More general: with weight function $w(x)$ in
  - original integral
  - $q(x)$ orthogonality
  - weights A_i

Numerical Quadrature—Summary

(n intervals)

	# func. evals	node placement	error $= 0\ \forall P_{\Box}$
CTR	$n+1$	uniform	1
CSR	$2n+1$	uniform	3
interp.	$n+1$	any (distinct)	n
GQ	$n+1$	zeros of $q(x)$	$2n+1$