Lecture 8: Integration

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Outline

Theorem (Fundamental Theorem of Calculus)

Let $f(x)$ be a real-valued function on a closed interval $[a, b]$ and let F be a continuous function on $[a, b]$ such that

$$F'(x) = f(x) \quad \text{on } (a, b).$$

If $f(x)$ is Riemann integrable on $[a, b]$, then

$$\int_a^b f(x)\,dx = F(b) - F(a).$$

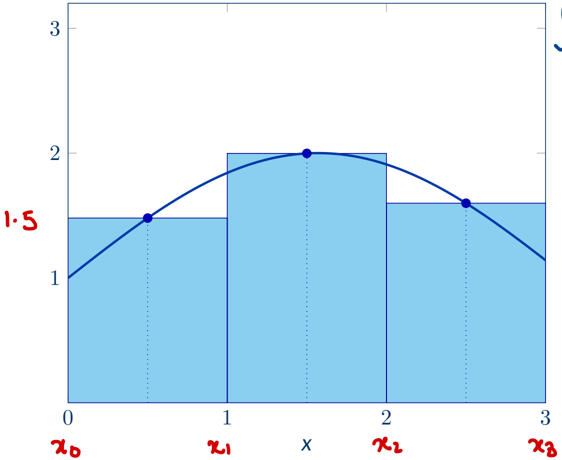


Figure 1: Riemann sum for a function $f(x)$.

$$\int_a^b f(x)\,dx \approx \overset{R}{\boxed{\sum_{i=0}^{n-1} (x_{i+1}-x_i) \times f(\xi_i)}}$$

for $\xi_i \in [x_i, x_{i+1}]$

Riemann Integration: For every $\varepsilon > 0$ $\exists$ $[x_{i-1}, x_i]$ partition of $[a,b]$ st.

$$\left| \int_a^b f(x)\,dx - R \right| < \varepsilon$$

$$f(x) \approx P_n^L(x) = \sum_{i=0}^{n} f_i \, L_i(x)$$

$$\Rightarrow \int_a^b f(x)\,dx \approx \int_a^b \sum_{i=0}^{n} \underbrace{f_i}_{\text{Constant}} L_i(x) = \sum_{i=0}^{n} f_i \underbrace{\int_a^b L_i(x)}_{a_i}$$

$$= \sum_{i=0}^{n} f_i \, a_i$$

$$\text{Error}(f) = \frac{1}{(n+1)!} \int_a^b \prod_{i=0}^{n} (x - x_i)\, f^{(n+1)}(\xi(x))\, dx.$$

Take $n=2$; such that $x_0 = a$; $x_1 = b$

$$P_1^{L}(x) = \frac{(x-x_1)}{x_0-x_1} f_0 + \frac{(x-x_0)}{x_1-x_0} f_1$$

$$\int_a^b f(x)\,dx \approx \int_a^b P_1^{L}(x)\,dx = \frac{f_0}{x_0-x_1}\int_a^b (x-x_1)\,dx + \frac{f_1}{x_1-x_0}\int_a^b (x-x_0)\,dx$$

$$= \frac{f_0}{a-b}\int_a^b (x-b)\,dx + \frac{f_1}{b-a}\int_a^b (x-a)\,dx$$

$$= \frac{(b-a)}{2}\left[f_0 + f_1\right] = \boxed{\frac{(b-a)}{2}\left[f(a)+f(b)\right]}$$

Error $= -\dfrac{(b-a)^3}{12} f^{(2)}(\xi(x))$ for $\xi(x) \in (a,b)$.

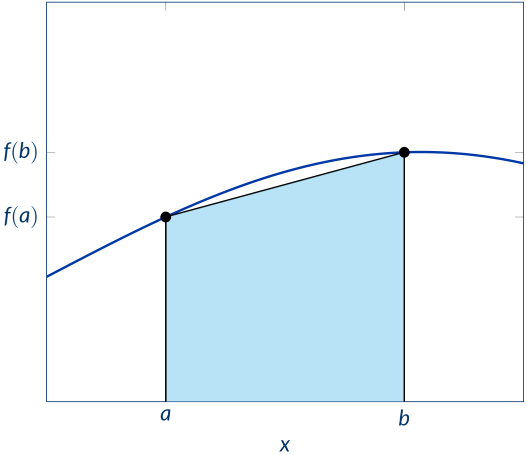


Figure 2: Trapezoidal rule for a function $f(x)$.

Example: $f(x)=x^2$ on $[0,2]$

$$I = \frac{(b-a)}{2}\left[f(a)+f(b)\right] = \frac{2}{2}[0+4] = 4.$$

$$\int_0^2 f(x)\,dx = \int_0^2 x^2\,dx = \left.\frac{x^3}{3}\right|_0^2 = \frac{8}{3}$$

$n=2$; $x_0 = a$, $x_1 = \frac{a+b}{2}$; $x_2 = b$

$$P_2^L(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f_0 + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f_1 + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f_2 .$$

$$I_S(f) = \frac{h}{3}\left[f_0 + 4f_1 + f_2\right] \quad \text{where } h = \frac{b-a}{2}$$

$$\boxed{= \frac{(b-a)}{6}\left[f_0 + 4f_1 + f_2\right]}$$

Example: $f(x) = x^2$ on $[0,2]$

$$I_S(f) = \frac{2}{6}\left[f(0) + 4f(1) + f(2)\right] = \frac{1}{3}\left[0 + 4 + 4\right] = \frac{8}{3}$$

$f(x) = x^3$; $= \frac{2}{6}\left[0 + 4 + 8\right] = \frac{12}{3} = 4$ $\quad \int_0^2 x^3\,dx = 4$

$f(x) = x^4$ $= \frac{2}{6}\left[0 + 4 + 16\right] = \frac{20}{3}$; $\int x^4 = 32/5$ $\times$

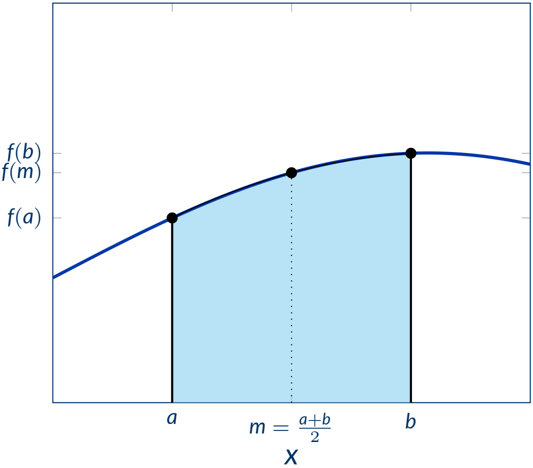


Figure 3: Simpson rule for a function $f(x)$.

DOP: The DOP of a ~~quadrature~~ integration formula is largest positive integer n s.t. formula is exact for x^k for $k = 0, 1, \dots, n$.

eg: Trapezoidal $= 1$

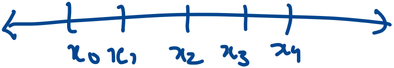
Simpson $= 3$.

Newton 3:8 rule $= 1$, $n = 3$;

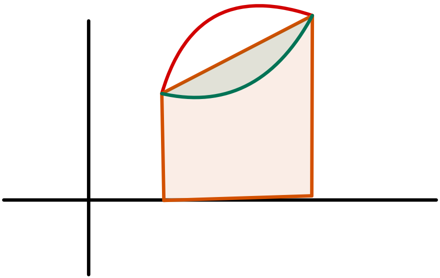
DOP $= 4$;

Bode : $n = 4$

DOP $= 4$



Gaussian Quadrature



Gaussian Quadrature computes integration on non-equally spaced points.

Here we approximate

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

where $\{c_i\}_{i=1}^{n}$; $\{x_i\}_{i=1}^{n}$ are unknowns.

$\hookrightarrow \in [a,b]$.

We have $2n$ unknowns $\Rightarrow$ Approximates a polynomial of degree $2n-1$.

Hence, n-point GQ gives exact integration for $2n-1$ degree polynomial.

Example

$n=2$; $[a,b]=[-1,1]$; $\{c_1, c_2, x_1, x_2\}$, $\underbrace{c_1 \neq 0,\ c_2 \neq 0}_{=0\text{'s then no contribution}}$, $\underbrace{x_1 \neq x_2}_{\text{same point}}$

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2)$$

This should be exact for degree 3 polynomials: i.e, $1, x, x^2, x^3$

$$\int_{-1}^{1} 1\,dx = c_1 + c_2 = 2$$

$$\int_{-1}^{1} x\,dx = c_1x_1 + c_2x_2 = 0$$

$$\int_{-1}^{1} x^2\,dx = c_1x_1^2 + c_2x_2^2 = 2/3$$

$$\int_{-1}^{1} x^3\,dx = c_1x_1^3 + c_2x_2^3 = 0$$

Easy

$c_1x_1 = -c_2x_2$

$\Rightarrow c_1x_1^3 + c_2x_2^3 = 0$

$\Rightarrow c_1x_1x_1^2 + c_2x_2^3 = 0$

$\Rightarrow -c_2x_2x_1^2 + c_2x_2^3 = 0$

$\Rightarrow x_2c_2(-x_1^2 + x_2^2) = 0$

$c_2 \neq 0$; $\quad x_1^2 = x_2^2 \Rightarrow x_1 = \pm x_2$

$\neq 0$ (?) Why $\quad x_1 \neq x_2$; $x_1 = -x_2$

$c_1 = c_2 = 1$; $\quad x_1 = \frac{-1}{\sqrt{3}}$, $x_2 = \frac{1}{\sqrt{3}}$

$$\int_{-1}^{1} f(x)\,dx \approx f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

In general to compute $\{c_i\}$, $\{x_i\}$, we use Legendre polynomials. They are defined over $[-1,1]$ and

Orthogonal polynomials

$$\int_{-1}^{1} p(x) P_n(x) = 0 \quad ; \text{ for every polynomial } p(x) \text{ of}$$

degree less than or equal to n.

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

$x=a$; $t=-1$

$x=b$; $t=1$

$$; \quad t = \frac{2x-a-b}{b-a} \quad ; \quad dt = \frac{2\,dx}{b-a}$$

$$\int_a^b f(x)\,dx = \left.\int_{-1}^{1} f\left(\frac{(b-a)t+(a+b)}{2}\right)\frac{(b-a)}{2}\,dt \right\} \rightarrow \text{GQ.}$$

Eigenvalue Problems :

Schrödinger Equation: Time-independent

$$\boxed{H|\psi\rangle = E\psi}$$

$$Ax = \lambda x$$

Maximum eigenvalue $\rightarrow |\lambda_{max}|$

Minimum eigenvalue $\rightarrow |\lambda_{min}|$