Lecture October 15

Numerical integration

Newton-Cotes quadrature

- Trapezoidal $(O(h^3))$
- Rectangular $(O(h^3))$
- Simpson's $(O(h^5))$

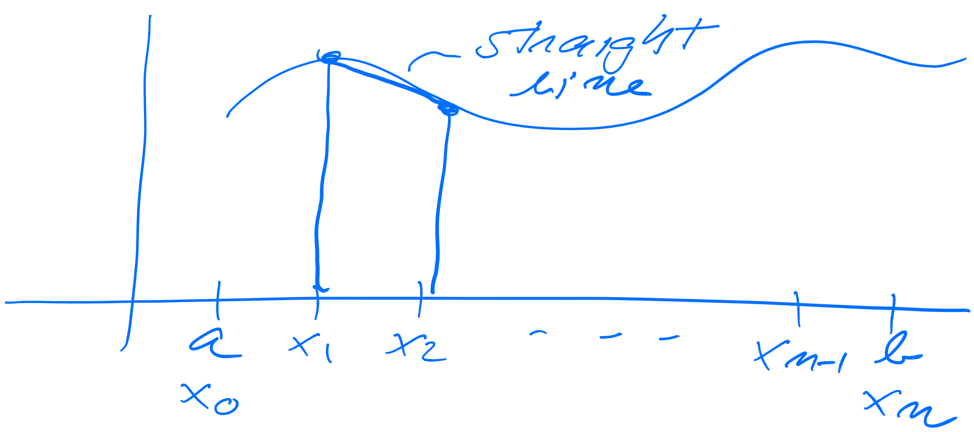
⋮

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

int. points (x_i), weights (w_i)

Trapezoidal:

$$w = \left\{\frac{h}{2}, h, h, \ldots, h, \frac{h}{2}\right\}$$



$$x_i = x_0 + i \cdot h \qquad i = 0, 1, 2, \ldots n$$

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

w_i = Defined by polynomial

approx.

with n points, can we approximate $f(x) \simeq P_{2n-1}(x)$?

Yes, $\Rightarrow$ Gaussian quadrature, usage of orthogonal polynomials?

Example: Legendre polynomials

$L_0(x) = 1$ $\qquad L_2(x) = \frac{1}{2}(3x^2 - 1)$

$L_1(x) = x$ $\qquad x \in [-1, 1]$

$$\int_{-1}^{1} L_i(x) L_j(x)\, dx = \frac{2}{2 \cdot i + 1} \delta_{ij}$$

orthogonal polynomials:

- integration points = zeros of an nth-order orthogonal polynomial,
- integration weights = inverse elements of a matrix containing the orthogonal polynomials.

$L_2(x)$: n-points $= 2$

$$f(x) \approx P_3(x)$$

$$L_2(x) = \frac{1}{2}(3x^2 - 1) = 0 \Rightarrow \boxed{\begin{aligned} x_0 &= -\frac{1}{\sqrt{3}} \\ x_1 &= \frac{1}{\sqrt{3}} \end{aligned}}$$

$$\boxed{w_0 = w_1 = 1}$$

$$\int_{-1}^{1} x^2 \, dx = I \qquad \boxed{n = 2}$$

$$= 2/3$$

Trapezoidal rule:

$$I_T \approx \sum_{i=0}^{1} w_i f(x_i) \qquad \begin{aligned} x_0 &= -1 \\ x_1 &= +1 \end{aligned}$$

$$= \frac{h}{2}[1 + 1] = h$$

$$h = \frac{1 - (-1)}{2} = 1$$

$$I_T = 1 \neq 2/3$$

$$I_{GLeg} = 1 \cdot \left(-\frac{1}{\sqrt{3}}\right)^2 + 1 \cdot \left(\frac{1}{\sqrt{3}}\right)^2$$

$$= 2/3$$

$$I = \int_a^b f(x)\,dx = \int_a^b W(x) g(x)\,dx$$

weight

weight
function

Example:

$$\int_0^\infty \underbrace{x^n e^{-x}} dx = n!$$

part of a specific orthogonal polynomial: Laguerre

$$\int_0^\infty x^n e^{-x} dx = \int_0^\infty W(x)\, dx$$

$$\underbrace{\int_0^\infty x^n e^{-x} g(x)\, dx}_{\text{Laguerre}} = \int_0^\infty W(x)\, g(x)\, dx$$

Laguerre $x \in [0, \infty)$

$$\int_{-\infty}^\infty \underbrace{e^{-x^2}} g(x)\, dx = \int_{-\infty}^\infty \underbrace{W(x)} g(x)\, dx$$

Hermite $x \in (-\infty, \infty)$

$$\int_0^\infty x e^{-x} dx = \underline{1}$$

$$\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} g(x)\,dx = \int_{-1}^{1} W(x) g(x)\,dx$$

Chebyshev $\in [-1,1]$

$$\int_a^b W(x) g(x)\,dx = \sum_{i=0}^{n-1} w_i\, g(x_i)$$

n-points :

$$f(x) \simeq P_{2n-1}(x)$$

$$\int_a^b f(x)\,dx \simeq \int_a^b P_{2n-1}(x)$$

$$\simeq \sum_{i=0}^{n-1} P_{2n-1}(x_i)\, w_i$$

$$P_{2n-1}(x) = L_n(x)\, P_{n-1}(x) + Q_{n-1}(x)$$

(using Legendre)

$$P_3(x) = 3x^3 + 5x^2 + 2 \qquad x \in [-1,+1]$$

$$\int_{-1}^{1} P_3(x)\,dx = 22/3 \qquad \boxed{n = 2}$$

$$L_n(x) = L_2(x) = (3x^2-1)/2$$

$$P_1(x) = (2x + 10/3)$$

$$Q_1(x) = x + 11/3$$

$$\int_{-1}^{1} P_3(x)\,dx = \underline{\int_{-1}^{1} L_2(x)\, P_1(x)\, dx} \overset{?}{=} 0$$

$$+ \int_{-1}^{1} Q_1(x)\, dx$$

$$P_1(x) = \sum_{i=0}^{1} a_i L_i(x) \qquad L_0(x) = 1, \quad L_1(x) = x$$

$$\int_{-1}^{1} P_3(x)\,dx = \int_{-1}^{1} Q_1(x)\,dx$$

General result:

$$\int_a^b P_{2n-1}(x)\,dx = \int_a^b Q_{n-1}(x)\,dx$$

$$\simeq \sum_{i=0}^{1} w_i\, P_3(x_i)\,dx = 22/3$$

$$w_0 = 1 = w_1$$

$$x_0 = -\frac{1}{\sqrt{3}} \qquad x_1 = \frac{1}{\sqrt{3}}$$

Specialize to [illegible]

$x \in [-1, +1]$

$$\int_{-1}^{1} f(x)\,dx \simeq \int_{-1}^{1} P_{2n-1}(x)\,dx$$

$$= \int_{-1}^{1} Q_{n-1}(x)\,dx$$

Expand $Q_{n-1}(x)$ in terms of L_i:

$$Q_{n-1}(x) = \sum_{i=0}^{n-1} \alpha_i L_i(x)$$

$$L_0(x) = 1$$

$$\int_{-1}^{1} Q_{n-1}(x)\,dx = \sum_{i=0}^{n-1} \alpha_i \underbrace{\int_{-1}^{1} 1 \cdot L_i(x)\,dx}_{?}$$

$$\int_{-1}^{1} L_0(x) L_i(x)\,dx$$

$$= \delta_{0i} \frac{2}{2i+1}$$

$$= 2\alpha_0$$

$$\int_{-1}^{1} f(x)\,dx \simeq \int_{-1}^{1} P_{2n-1}(x)\,dx = 2\alpha_0$$

$$Q_{n-1}(x_k) = \sum_{i=0}^{n-1} \alpha_i L_i(x_k)$$

$x_k \quad k = 0, 1, \dots n-1$

are the zeros of the Legendre polynomial L_n

$$L_n(\underline{x_k}) = 0$$

$$P_{2n-1}(x_k) = \underbrace{L_n(x_k)}_{=0} P_{n-1}(x_k) + Q_{n-1}(x_k)$$

$$P_{2n-1}(x_k) = Q_{n-1}(x_k)$$

$$\mathbb{L} = \begin{bmatrix} L_0(x_0) & L_1(x_0) & \dots & L_{n-1}(x_0) \\ L_0(x_1) & L_1(x_1) & - & - \\ \vdots & & & \\ L_0(x_{n-1}) & - & - & L_{n-1}(x_{n-1}) \end{bmatrix}$$

$$\mathbb{L}^{-1}\mathbb{L} = \mathbb{1}$$

$$Q_{n-1}(x_0) = \alpha_0 L_0(x_0) + \alpha_1 L_1(x_0) + \dots$$

$$Q_{n-1}(x_1) = \alpha_0 L_0(x_1) + \alpha_1 L_1(x_1) + \dots$$

$\vdots$

$$q_{n-1}(x_{n-1}) = \alpha_0 l_0(x_{n-1}) + \dots$$

$$Q_{n-1} = [q_{n-1}(x_0), q_{n-1}(x_1) \dots]^T$$

$$\alpha = [\alpha_0, \alpha_1 \dots \alpha_{n-1}]^T$$

$$Q_{n-1} = L\alpha \quad \Rightarrow$$

$$\alpha = L^{-1} Q_{n-1}$$

$$\alpha_k = \sum_{i=0}^{n-1} (L^{-1})_{ki} \, q_{n-1}(x_i)$$

$$\int_{-1}^{1} P_{2n-1}(x)\,dx = \int_{-1}^{1} q_{n-1}(x)\,dx$$

$$= 2\alpha_0 = \sum_{i=0}^{n-1} (L^{-1})_{0i} \, q_{n-1}(x_i)$$

$$= \sum_{i=0}^{n-1} \underline{(L^{-1})_{0i}} \, P_{2n-1}(x_i)$$

Exact

$$= \sum_{i=0}^{n-1} w_i \, \underbrace{P_{2n-1}(x_i)}_{\simeq f(x_i)}$$

$$\simeq \sum_{i=0}^{n-1} w_i \, f(x_i)$$

$$i=0$$

Example : $n = 2$

$$L_2(x) = \frac{1}{2}(3x^2 - 2)$$

$$x_0 = -\frac{1}{\sqrt{3}} \quad \wedge \quad x_1 = +1/\sqrt{3}$$

$$Q_{n-1}(x_k) = \sum_{i=0}^{n-1} \alpha_i L_i(x_k)$$

$$\left[\begin{array}{l} Q_1(x_0) = \alpha_0 - \alpha_1 \frac{1}{\sqrt{3}} \qquad L_1 = x \\ Q_1(x_1) = \alpha_0 + \alpha_1 \frac{1}{\sqrt{3}} \end{array}\right.$$

$$L = \begin{bmatrix} 1 & -1/\sqrt{3} \\ 1 & +1/\sqrt{3} \end{bmatrix}$$

$$Q_1 = L \cdot \alpha \qquad \alpha = [\alpha_0, \alpha_1]^T$$

$$L^{-1} = \frac{\sqrt{3}}{2} \begin{array}{c} \begin{array}{cc} w_0 & \quad w_1 \end{array} \\ \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{3} \\ -1 & 1 \end{bmatrix} \end{array}$$

$$w_0 = \underline{1} \qquad\qquad w_i = \underline{2}(L^{-1})_{0i}$$

$$w_1 = \underline{1}$$