Quadrature: Given $f \in C([-1,1])$. $I = \int_{-1}^{1} f(x)\,dx = ?$

Distinct nodes $x_0, \dots, x_n \in [-1,1]$; weights $w_0, \dots, w_n \in [-1,1]$.

$I \approx I_n = \sum_{k=0}^{n} w_k f(x_k)$. Usually $\{w_k\}$ come from poly. interp.

That is $$\int_{-1}^{1} f(x)\,dx \approx \int_{-1}^{1} \underset{\substack{\uparrow \\ \text{poly. interp.} \\ \text{of } f.}}{p_n(x)}\,dx = \sum_{k=0}^{n} w_k p(x_k) = \sum_{k=0}^{n} w_k f(x_k).$$

Three quadrature rules

① Newton-Cotes : $\{x_j\}$ equispaced pts. $|I - I_n|$ can diverge as $n \to \infty$. [Pölya, 1933].

② Clenshaw-Curtis : $\{x_j\}$ = chebyshev pts.

③ Gauss quadrature : $\{x_j\}$ = Legendre pts, i.e., $\underset{\substack{\uparrow \\ \text{Legendre poly.}}}{P_{n+1}}(x_j) = 0$.

Thm 19.1: For any quadrature rule from poly. interpolants,

$I = I_n$ if $f \in \mathcal{P}_n$

For Gauss, $I = I_n$ if $f \in \mathcal{P}_{2n+1}$.

Proof: If $f \in \mathcal{P}_{2n+1}$, then $f(x) = q_n(x) P_{n+1}(x) + r_n(x)$ $r_n, q_n \in \mathcal{P}_n$.

$$I = \int_{-1}^{1} f(x)\,dx = \underbrace{\int_{-1}^{1} q_n(x) P_{n+1}(x)}_{\substack{=0 \\ \text{by orthogonality}}} + \int_{-1}^{1} r_n(x)\,dx = \sum_{k=0}^{n} w_k r_n(x_k)$$

Also, $f(x_j) = \underbrace{q_n(x_j) P_{n+1}(x_j)}_{=0} + r_n(x_j) = r_n(x_j)$.

So, $\quad I = \int_{-1}^{1} f(x)\,dx = \sum_{k=0}^{n} w_k f(x_k)$.

<u>Implementation</u> - Clenshaw - Curtis

$$\int_{-1}^{1} T_k(x)\,dx = \begin{cases} 0 & \text{if } k \text{ is odd} \\ \frac{2}{1-k^2} & \text{if } k \text{ is even.} \end{cases}$$

<u>Algorithm</u>:

$$\int_{-1}^{1} f(x)\,dx \approx \int_{-1}^{1} \sum_{k=0}^{n} c_k T_k(x)\,dx = \sum_{k=0}^{n} c_k \int_{-1}^{1} T_k(x)\,dx$$

$\uparrow$ get via DCT.

$$= \sum_{k=0}^{\lfloor n/2 \rfloor} c_{2k} \frac{2}{1-(2k)^2}.$$

Clenshaw - Curtis can also be written as $\int_{-1}^{1} f(x)\,dx \approx \sum_{k=0}^{n} w_k f(x_k)$.

<u>Implementation</u> - Gauss

[Golub - Welsch 1969] $\qquad \{x_j\}$ = Legendre pts: $P_{n+1}(x_j) = 0$.

<u>Idea</u>: Find roots of $P_{n+1}(x) = 0$ by eigenvalue problem.

$$P_0(x) = 1, \quad P_1(x) = x$$
$$(n+1) P_{n+1}(x) = (2n+1)\, x\, P_n(x) - n P_{n-1}(x), \quad n \geq 1.$$

$$\begin{bmatrix} 0 & 1 & & & \\ \frac{1}{3} & 0 & \frac{2}{3} & & \\ & \frac{2}{5} & 0 & \frac{3}{5} & \\ & & \ddots & \ddots & \ddots \\ & & & \frac{n}{2n+1} & 0 \end{bmatrix} \begin{bmatrix} P_0(\lambda) \\ \vdots \\ P_n(\lambda) \end{bmatrix} = \lambda \begin{bmatrix} P_0(\lambda) \\ \vdots \\ P_n(\lambda) \end{bmatrix}$$

Find eigenvalues of this!

Accuracy: How small is $E_n(f) = I_n - I$. ?

~~Clenshaw Curtis~~:

f = Lipshitz cont. $\quad f(x) = \sum_{k=0}^{\infty} a_k T_k(x)$.

So: $\quad E_n(f) = \sum_{k=0}^{\infty} a_k E_n(T_k) = \sum_{\substack{k=0 \\ k=\text{even}}}^{\infty} a_k E_n(T_k)$

CC: $\quad E_n(f) = \sum_{\substack{k=n+1 \\ k=\text{even}}}^{\infty} a_k E_n(T_k)$, Gauss: $E_n(f) = \sum_{\substack{k=2n+2 \\ k=\text{even}}}^{\infty} a_k E_n(T_k)$.

Suppose f = analytic in Bernstein ellipse with $\rho > 1$, with $|f(x)| \le M$

Then, $|a_k| \le 2M\rho^{-k}$.

CC:
$$|E_n(f)| \le \sum_{\substack{k=n+1 \\ k=\text{even}}}^{\infty} |a_k|\,|E_n(T_k)|$$
$$\le \sum_{\substack{k=n+1 \\ k=\text{even}}}^{\infty} 2M\rho^{-k} \, |E_n(T_k)|$$
$$\le 8M \frac{\rho^{-n-1}}{1-\rho^{-2}}.$$

Gauss:
$$|E_n(f)| \le \frac{8M\rho^{-2n-2}}{1-\rho^{-2}}.$$

Quadrature $\longleftrightarrow$ rational functions

$$I = \int_{-1}^{1} f(x)\,dx, \qquad I_n = \sum_{k=0}^{n} w_k f(x_k).$$

Claim: Every quadrature can be thought of as:

1. Approximate $f(x)$ by rational interpolant.
2. Integrate rational interpolant exactly.

Let $\int_{-1}^{1} f(x)\,dx \approx \sum_{k=0}^{n} w_k f(x_k)$.

Take $r(x) = \dfrac{p(x)}{q(x)}$ where p and q are of degree $\leq n$.

so that $r(x_j) = f(x_j)$.

LAGRANGE FORM:

Lagrange func. $\ell(x) = (x - x_0)\cdots(x - x_n)$.

Lagrange weights $v_k = \dfrac{1}{\prod_{\substack{i=0\\ i\neq k}}^{n} (x_k - x_i)}$

$$q(x) = \ell(x) \sum_{k=0}^{n} \frac{v_k}{x - x_k} q(x_k)$$

$\left\{\begin{array}{l} \text{Pf: } \cdot \text{ rhs is a poly. of deg} \leq n. \\ \cdot \text{ rhs interpolants } q(x) \text{ at } x_k. \end{array}\right.$

We know that $q(x_j)\, r(x_j) = p(x_j)$.

Therefore $$p(x) = \ell(x) \sum_{k=0}^{n} \frac{v_k}{x - x_k} q(x_k)\, r(x_k).$$

Hence,

$$r(x) = \frac{p(x)}{q(x)} = \frac{\displaystyle\sum_{k=0}^{n}{}' \frac{\mu_k r(x_k)}{x - x_k}}{\displaystyle\sum_{k=0}^{n}{}' \frac{\mu_k}{x - x_k}} \qquad \mu_k = v_k q(x_k).$$

Therefore,

$$\int_{-1}^{1} f(x)\,dx \approx \int_{-1}^{1} r(x)\,dx = \int_{-1}^{1} \frac{\displaystyle\sum_{k=0}^{n}{}' \frac{\mu_k r(x_k)}{x - x_k}}{\displaystyle\sum_{k=0}^{n}{}' \frac{\mu_k}{x - x_k}}\,dx$$

$$= \sum_{k=0}^{n}{}' \Bigg(\underbrace{\int_{-1}^{1} \frac{\left(\frac{\mu_k}{x - x_k}\right)}{\displaystyle\sum_{k=0}^{n}{}' \frac{\mu_k}{x - x_k}}\,dx}_{= w_k} \Bigg) r(x_k)$$

* If you want to understand a quadrature rule, then first understand what rational interpolant it is building.

Example: Monte Carlo:

① Sample $f(x)$ at $x_0, \dots, x_n$ (random locations)

② Take $\displaystyle\int_{\Omega} f(\underline{x})\,d\underline{x} = |\Omega| \frac{1}{n+1} \sum_{k=0}^{n}{}' f(x_k)$.

vol. of Ω.

Equivalent to:

① Approximate $f(x)$ by a constant (using LS).

② Integrate constant exactly.

① Solve $\underbrace{\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}}_{A} c = \underbrace{\begin{bmatrix} f(x_0) \\ \vdots \\ f(x_n) \end{bmatrix}}_{\underline{b}}$ in least squares sense.

$A^T A = n+1$. $A^T b = \sum_{k=0}^{n} f(x_k)$. $A^T A c = A^T b$

so $c = \frac{1}{n+1} \sum_{k=0}^{n} f(x_k)$.

② Integrate const. exactly:

$$\int_\Omega f(\underline{x})\, d\underline{x} \approx \int_\Omega c\, d\underline{x} = |\Omega| \cdot \frac{1}{n+1} \sum_{k=0}^{n} f(x_k)$$

Understand $f(\underline{x}) \approx c$ by least squares...

High-order Monte Carlo in 1D

①
$$\begin{bmatrix} 1 & x_0 & x_0^2 \\ \vdots & \vdots & \vdots \\ 1 & x_N & x_N^2 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} f(x_0) \\ \vdots \\ f(x_N) \end{bmatrix}$$

2 Integrate $c_0 + c_1 x + c_2 x^2$ exactly.