Numerical Integration

Def: (Quadrature formula) $\sum_i w_i f(x_i) =: Q_a^b(f) \approx \int_a^b f(x)\,dx$

„weights“ „points“

Def (Closed Newton-Cotes) idea: use polynomial interpol. (Lagrange)

$$\int f(x)dx \approx \int p(x)dx = \int \sum f(x_i)\,\ell_i(x)\,dx = \sum f(x_i)\cdot \underbrace{\int \ell_i(x)\,dx}_{=w_i} =: Q^{CNC}(f)$$

where $x_i = \frac{i}{n}$, $i = 0, \dots n$

Def (Open-NC) here: $x = \frac{2i+1}{2n+2}$, $i = 0, \dots n$ (endpoints not included)

Theorem (NC-Accuracy): n odd: exact for $f \in P_n$

n even: exact for $f \in P_{n+1}$

No Proof

Definition $n = 1 \Rightarrow w_1 = \frac{1}{2}$, $w_2 = \frac{1}{2}$ $\Rightarrow$ „Trapezoidal-rule“: $T(f)$

$n = 2 \Rightarrow w_1 = \frac{1}{6} = w_3$, $w_2 = \frac{4}{6}$ $\Rightarrow$ „Simpson-rule“: $S(f)$

Theorem (Error of Trapezoidal rule)

(i) $f \in C([a,b]) \Rightarrow \left|\int_a^b f(x)dx - T(f)\right| \leq 2\sum_i h_i \min_{v \in P_1} \|f - v\|_\infty$

(ii) $f \in C^2([a,b]) \Rightarrow \left|\int f(x)dx - T(f)\right| \leq \frac{1}{4}\sum_i h_i^3 \|f^{(2)}\|_\infty \leq \frac{1}{4}(b-a)h^2 \|f^{(2)}\|_\infty$

$h = \max_i [h_i]$

Proof:

(i) $\int_{x_i}^{x_{i+1}} f(x)dx - T(f) = \int f(x) + v - v - T(f)\,dx = \int f - v\,dx - T(f-v)$

$\Rightarrow \left|\int_{x_i}^{x_{i+1}} f\,dx - T(f)\right| \leq h_i \|f - v\|_\infty + |T(f-v)|$

$\leq h_i \|f-v\|_\infty + h_i \|f - v\|_\infty = 2h_i \|f-v\|_\infty$

$\Rightarrow \left|\int_a^b f\,dx - T(f)\right| \leq \sum_i 2h_i \min_{v \in P_1} \|f - v\|_\infty$

(ii) Interpol. error $\Rightarrow \min_{v \in P_1} \|f - v\|_\infty \leq \frac{1}{8} h_i^2 \|f''\|_\infty \Rightarrow \left|\int f\,dx - T(f)\right| \leq \frac{1}{4}\sum_i h_i^3 \|f^{(2)}\|$

$\Rightarrow \left|\int_a^b f\,dx - T(f)\right| \leq \frac{1}{4} h^2 \|f''\|_\infty (b-a)$ ■

Remark: (Romberg Exrapolation) accelerate converg. of composite rules

As $\left| \int_a^b f\, dx - T_i(f) \right| \xrightarrow{N\to\infty} 0 \implies (h_i, T(h_i))$ with $h_i = \frac{b-a}{2^i}$

can be Neville-extrapolated.

As $T = \int f dx + c_1 h^2 + c_2 h^4 + \dots \implies$ use extrapol of $(h_i^2, T(h_i))$

Remark (Non-smooth Integrands & adaptivity)

$$f(x) = x^{0,1} \implies \mathcal{O}(h^{1,1}) \text{ not } \mathcal{O}(h^2) \text{ with Trapez.}$$

For this f, we get $\mathcal{O}(h^2)$ integration by:

1. equidist. points $x_i = \frac{i}{N}$
2. refine points "at" $x=0$: $x_i = \left(\frac{i}{N}\right)^{\beta}$

but for general f, difficult to construct.

Theorem (Legendre Polynomials)

A) $\exists$ unique sequence $L_n \in \mathcal{P}_n$ st.

i) $\{L_n\}$ is a basis for $\mathcal{P}_n$ $\forall n$

ii) L_n is orthog. to $\mathcal{P}_{n-1}$, ie $\langle L_n, v \rangle = 0$, $v \in \mathcal{P}_{n-1}$

iii) $L_n(1) = 1$

iv) L_{n+1} has $n+1$ zeros x_i, $x_i \in (-1, 1)$

B) ..

C) Recursion formula: $(n+1) L_{n+1}(x) = (2n+1) x L_n(x) - n L_{n-1}(x)$

Proof of A): use Gram Schmidt

Definition (Gauss Quadrature) idea: interpolate in zeros of L_n and integrate

$$Q^{Gauss}(f) := \sum_{i=0}^{n} w_{i,n}^G f(x_{i,n}^G), \quad w_{i,n} = \int_{-1}^{1} \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_{j,n}^G}{x_{i,n}^G - x_{j,n}^G} dx$$

zeros of L_{n+1}

Theorem (Gauss Q. exact for $f \in \mathcal{P}_{2n+1}$)

i) Q is exact for $f \in \mathcal{P}_{2n+1}$

iii) $w_{i,n}^G > 0$

ii) there is <u>no</u> quadrature that is exact for $f \in \mathcal{P}_{2n+2}$

Proof: i) $f \in \mathcal{P}_{2n+1}$

use Polynomial division to rewrite

$$f(x) = L_{n+1}(x)\, q_n(x) + r_n(x), \qquad q_n, r_n \in \mathcal{P}_n$$

$$\Rightarrow \int_{-1}^{1} f\, dx = \int \underbrace{L_{n+1}\, q_n}_{=0 \text{ (orthogonal)}} + r_n\, dx = Q^{Gauss}(r_n) = \sum_i w_{i,n}^G \cdot r_n(x_{i,n}^G)$$

$$= \sum w_{i,n} \left[r_n(x_{i,n}) + \underbrace{L_{n+1}(x_{i,n}) \cdot q_n(x_{i,n})}_{=0 \text{ (zeros of } L_n)} \right] = Q_n^{Gauss}(f)$$

ii)
iii) } No proofs

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Theorem (convergence/error of Gauss Q)

$$f \in C([-1,1]): \qquad \left| \int_{-1}^{1} f\, dx - Q^{Gauss}(f) \right| \leq 4 \min_{v \in \mathcal{P}_{2n+1}} \| f - v \|_\infty$$

Proof: $\left| \int f\, dx - Q(f) \right| = \left| \int f - v\, dx + Q(v) - Q(f) \right| = \left| \int f - v\, dx + Q(f-v) \right|$

$$\leq \left| \int f - v\, dx \right| + \left| Q(f-v) \right|$$

$$\leq 2 \cdot \| f - v \|_\infty + \sum_i \left| \underbrace{w_{i,n}}_{\geq 0} \right| \cdot \left| f(x^G) - v(x^G) \right|$$

$$\leq \Big[2 + \underbrace{\sum w_{i,n}^G}_{=2} \Big] \cdot \| f - v \|_\infty = 4 \cdot \| f - v \|_\infty$$

■

Remark (Composite Gauss vs. Trapez.)

Comp. Gauss conv. faster than Comp. Trap.
except for smooth, periodic functions!

Definition (Quadrature in 2D on Square)

$$Q := \sum_{ij} w_i w_j F(x_i, x_j) \quad \text{s.t. it is exact}$$

for polynomials $F \in \text{span}\{ x^i y^j : i,j = 0, \dots p \}$

Definition (Q. in 2D on Triangle)

- either: select some points on T, determine weights s.t. certain polynom. are integrated exactly
- or: change of variables to square

Remark (solve Gauss Q.) 2 options:

1. Newton method $\Rightarrow$ zeros of L_n, init guess: zeros of Chebyshev-polynom.
2. compute zeros of L_n as eigenvalues of certain matrix

Lemma (zeros of L_n as eigenvalues) $L_0 = 1,\ L_1 = x,\ L_n = (a_n x + b_n) L_{n-1} - c_n L_{n-1}$

$\Rightarrow$ zeros of L_n are ev of $J \in \mathbb{R}^{n \times n}$

Proof: rewrite recurrence relation:

$$x \cdot \begin{pmatrix} L_0 \\ \vdots \\ L_{n-1} \end{pmatrix} = \underbrace{\begin{pmatrix} -\frac{b_1}{a_1} & \frac{1}{a_1} & & \\ \frac{c_2}{a_2} & \ddots & \ddots & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix}}_{=:T} \cdot \begin{pmatrix} L_0 \\ \vdots \\ L_{n-1} \end{pmatrix} + \begin{pmatrix} 0 \\ \vdots \\ \vdots \\ \frac{1}{a_1} L_n \end{pmatrix}$$

$\Leftrightarrow \quad x \cdot \vec{L} = T\vec{L} + \frac{1}{a_n} L_n \vec{e}_n$

$\Rightarrow \quad \vec{L}_\xi := (L_0(\xi), \dots L_{n-1}(\xi))^T$ is an ev of T iff. $L_n(\xi) = 0$

$\Rightarrow \quad$ ev of T are zeros of of L_n with evec $\vec{L}_\xi$

$J := DTD^{-1}$, $D = \mathrm{diag}(d_0, \dots d_{n-1})$ ... J is symm.

ev of J = ev of T and evec of J: $v_i = d_i \cdot \vec{L}_\xi$ ... orthogonal

Lemma (Quadrature weights) given evec of J: $\vec{v}_i$ .. basis of $\mathbb{R}^n$

$$\Rightarrow w_i \vec{v}_i^T \vec{v}_i = \int_{-1}^{1} L_0^2(x)\,dx = 2\left[(\vec{v}_i)_1\right]^2$$

Proof: exactness $\Leftrightarrow$ $f \in \mathcal{P}_{n-1}$: $\sum w_j f(x_j) = \int f(x)\,dx$

choose $f := d_i L_i(x) \Rightarrow \sum w_j d_i L_i(x) = \int d_i L_i(x)\,dx = \int d_i \overbrace{\underbrace{L_0}_{=1} L_i}^{\text{orthog.}}\,dx$

$$= \delta_{i0} d_i \|L_0\|_{L^2}^2 = 2 d_i \delta_{i0}$$

rewrite using $V := (\vec{v}_0, \dots \vec{v}_{n-1})$, $\vec{w} := (w_0, \dots w_{n-1})^T$

$$V\vec{w} = 2 d_i \vec{e}_1 \qquad \Big| \cdot \vec{v}_i^T$$

$$\Rightarrow \quad \vec{v}_i^T \vec{v}_i w_i = \dots = 2\left[(v_i)_1\right]^2$$

Theorem (generalized Gauss Q.) [redacted] If func $w > 0$, $\int_{-1}^{1} w\,dx < \infty$, weights $w_i > 0$ s.t.

$$\int_{-1}^{1} f(x) w(x)\,dx = \sum w_i f(x_i) \quad \forall f \in \mathcal{P}_{2n+1}$$

$\Rightarrow$ x_i are zeros of polynomials, that are orthog. wrt. $\langle u, v \rangle = \int u v w(x)\,dx$

$\Rightarrow$ $w \equiv 1$: Legendre polyn.
$w = (1-x^2)^{-1}$: Chebyshev poly