

Numerical Methods for Computational Science and Engineering

Prof. R. Hiptmair, SAM, ETH Zurich

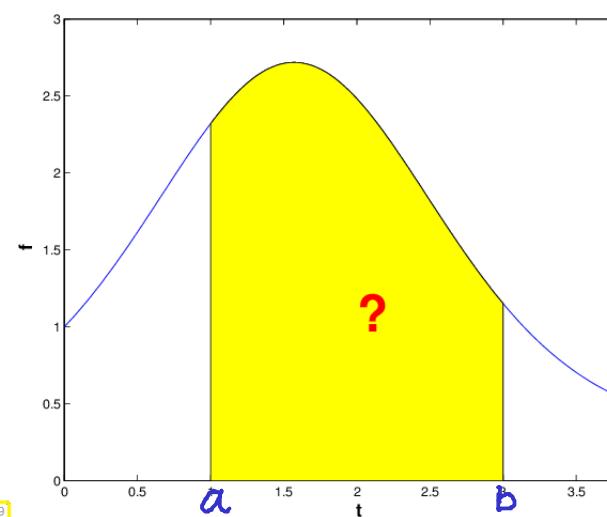
(with contributions from Prof. P. Arbenz and Dr. V. Gradinaru)

Autumn Term 2016

(C) Seminar für Angewandte Mathematik, ETH Zürich

URL: <http://www.sam.math.ethz.ch/~hiptmair/tmp/NumCSE/NumCSE16.pdf>

VII. Numerical Quadrature



Approximate $\int_a^b f(t) dt$
only point evaluations possible

Application :

assume time-harmonic periodic excitation with period $T > 0$.

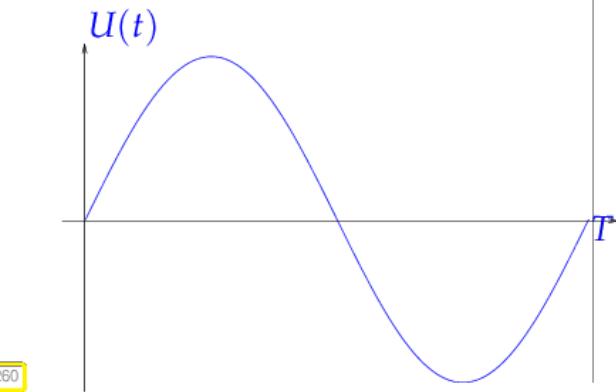


Fig. 260

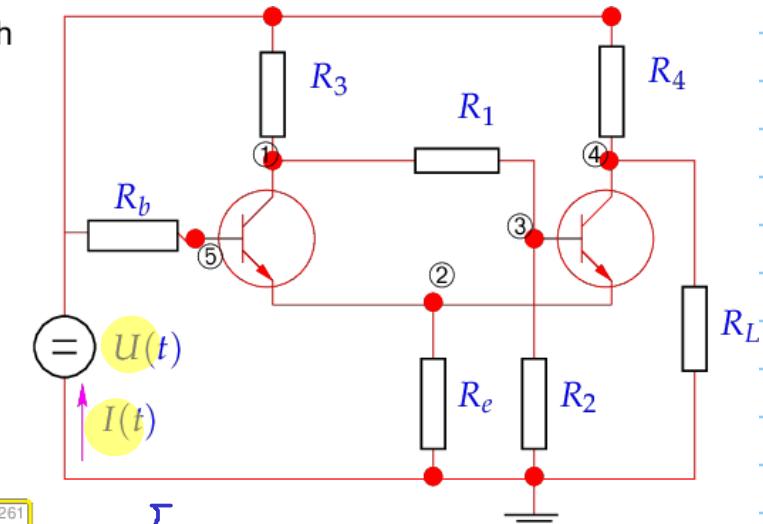


Fig. 261

$$\text{Total heat generation : } W = \int_0^T U(t) I(t) dt$$

↑
output of "black box" function

5.1. Quadrature formulas

Definition 7.1.1. Quadrature formula/quadrature rule

An n -point quadrature formula/quadrature rule on $[a, b]$ provides an approximation of the value of an integral through a weighted sum of point values of the integrand:

$$\int_a^b f(t) dt \approx Q_n(f) := \sum_{j=1}^n w_j f(c_j). \quad (7.1.2)$$

↑ weight
↑
 $c_j \in [a, b] \equiv$ nodes
 $\text{cost}(Q.F.) = \# f\text{-evaluation} = n$

②

Given: Q.F. $(\hat{w}_j, \hat{c}_j)_{j=1}^n$ on $[-1, 1]$ (reference interval)

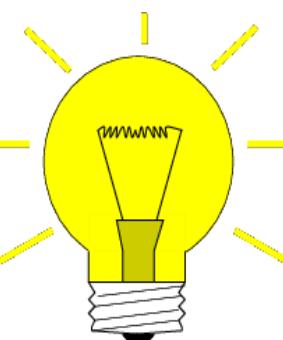
$$\Phi : [-1, 1] \rightarrow [a, b], \quad \Phi(\tau) = a + \frac{1}{2}(b-a)(\tau+1)$$

$$\int_a^b f(t) dt = \int_{-1}^1 f(\Phi(\tau)) \left| \frac{d\Phi}{d\tau}(\tau) \right| d\tau = \frac{1}{2}(b-a) \int_{-1}^1 f(\Phi(\tau)) d\tau$$

$$\approx \frac{1}{2}(b-a) \sum_{j=1}^n \hat{w}_j f(\Phi(\hat{c}_j))$$

Apply Q.F.

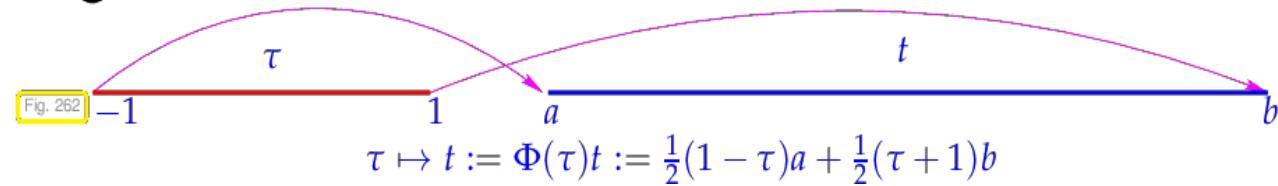
Q.F. on $[a, b]$



Idea: transformation formula for integrals

$$\int_a^b f(t) dt = \frac{1}{2}(b-a) \int_{-1}^1 \hat{f}(\tau) d\tau, \quad (7.1.5)$$

$$\hat{f}(\tau) := f\left(\frac{1}{2}(1-\tau)a + \frac{1}{2}(\tau+1)b\right).$$



quadrature formula for general interval $[a, b], a, b \in \mathbb{R}$:

$$\int_a^b f(t) dt \approx \frac{1}{2}(b-a) \sum_{j=1}^n \hat{w}_j \hat{f}(\hat{c}_j) = \sum_{j=1}^n w_j f(c_j) \quad \text{with} \quad c_j = \frac{1}{2}(1-\hat{c}_j)a + \frac{1}{2}(1+\hat{c}_j)b, \\ w_j = \frac{1}{2}(b-a)\hat{w}_j.$$

In codes: tabulated quadrature formula

```
struct QuadTab {
    template <typename VecType>
    static void getrule(int n, VecType &c, VecType &w,
                        double a=-1.0, double b=1.0);
}
```

Quadrature by interpolation:

space of simple functions
↓

Interpolation scheme: $I_J : \begin{cases} J \subset [a, b] \\ \int_a^b f(t) dt \end{cases} \approx \int_a^b (I_J[f(t_j)])_{j=0}^n (\tau) d\tau$

If I_J is linear
 $= \sum_{j=0}^n f(t_j) \int_a^b I_J(e_j)(\tau) d\tau$
(*) nodes J-th unit vector

weight w_j
↳ depend only on I_J

(3)

Quadrature error :

$$E_n(f) = \left| \int_a^b f(t) dt - Q_n(f) \right|$$

Our focus: n -dependence of $E_n(f)$ for families of Q.F. (for $n \rightarrow \infty$)

↳ "Asymptotic convergence"

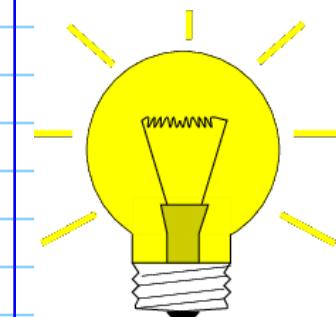
If Q.F. induced by $I_{\mathcal{T}}$

$$\begin{aligned} E_n(f) &= \left| \int_a^b (f - I_{\mathcal{T}}[f(t_j)]_j)(t) dt \right| \\ &\leq |b-a| \cdot \|f - I_{\mathcal{T}}[f(t_j)]_j\|_{\infty, [a,b]} \end{aligned}$$

↑
interpolation error
[→ Chapter 6!]

5.2. Polynomial Quadrature Formulas

→ Now: $I_{\mathcal{T}} \equiv$ Lagrange interpolation



Idea: replace integrand f with $p_{n-1} := l_{\mathcal{T}} \in \mathcal{P}_{n-1}$ = polynomial Lagrange interpolant of f (\rightarrow Cor. 5.2.15) for given node set $\mathcal{T} := \{t_0, \dots, t_{n-1}\} \subset [a, b]$

► $\int_a^b f(t) dt \approx Q_n(f) := \int_a^b p_{n-1}(t) dt . \quad (7.2.1)$

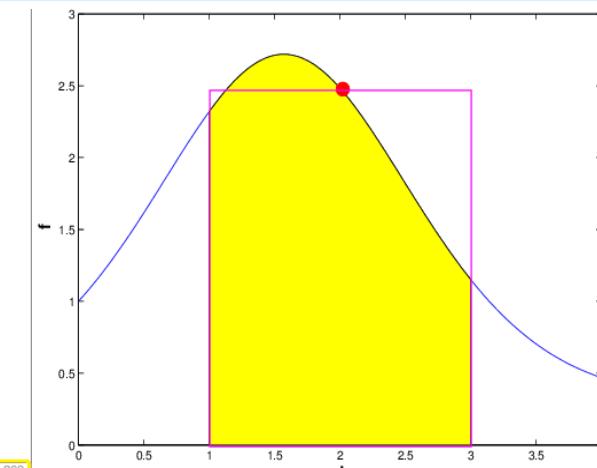
$$\sum_{j=0}^n f(t_j) \int_a^b I_{\mathcal{T}}(e_j)(t) dt$$

If $I_{\mathcal{T}} \equiv$ Lagrange interpolation :

$$I_{\mathcal{T}}(e_j) = L_j : \text{Lagrange pols.}$$

Examples :

$n=1$:



The midpoint rule is (7.2.2) for $n = 1$ and $t_0 = \frac{1}{2}(a+b)$. It leads to the 1-point quadrature formula

$$\int_a^b f(t) dt \approx Q_{mp}(f) = (b-a)f\left(\frac{1}{2}(a+b)\right).$$

"midpoint"

▷ the area under the graph of f is approximated by the area of a rectangle.

④

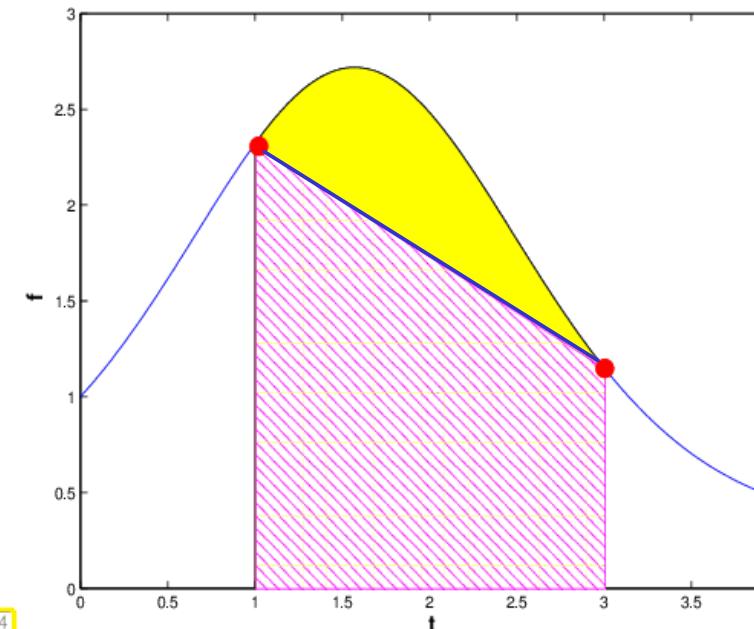
 $n=2:$

trapezoidal rule:

> trapez := newtoncotes(1);

$$\hat{Q}_{\text{trp}}(f) := \frac{1}{2}(f(0) + f(1)) \quad (7.2.5)$$

$$\left(\int_a^b f(t) dt \approx \frac{b-a}{2} (f(a) + f(b)) \right)$$

Newton-Cotes Q.F.: equidistant nodes $t_j = a + \frac{j}{n-1}(b-a)$

↳ unstable for large $n!$ $j=0, \dots, n-1$

Better: Chebyshev nodes \rightarrow Clenshaw-Curtis Q.F.

5.3. Gauss Quadrature

Gauging "quality" of Q.F.

Definition 7.3.1. Order of a quadrature rule
The **order** of quadrature rule $Q_n : C^0([a, b]) \rightarrow \mathbb{R}$ is defined as

$$\text{order}(Q_n) := \max\{m \in \mathbb{N}_0 : Q_n(p) = \int_a^b p(t) dt \quad \forall p \in \mathcal{P}_m\} + 1, \quad (7.3.2)$$

that is, as the **maximal** degree +1 of polynomials for which the quadrature rule is guaranteed to be exact.▷ Polynomial Q.F. with n points \Rightarrow order n
Theorem 7.3.5. Sufficient order conditions for quadrature rules
An n -point quadrature rule on $[a, b]$ (\rightarrow Def. 7.1.1)

$$Q_n(f) := \sum_{j=1}^n w_j f(t_j), \quad f \in C^0([a, b]),$$

with nodes $t_j \in [a, b]$ and weights $w_j \in \mathbb{R}, j = 1, \dots, n$, has **order $\geq n$** , if and only if

$$w_j = \int_a^b L_{j-1}(t) dt, \quad j = 1, \dots, n,$$

where $L_k, k = 0, \dots, n-1$, is the k -th **Lagrange polynomial** (5.2.11) associated with the ordered node set $\{t_1, t_2, \dots, t_n\}$.

$$L_{j-1}(t_e) = \delta_{j,e} \Rightarrow \int_a^b L_{j-1}(t) dt = Q_n(L_{j-1})$$

$L_{j-1} \in \mathcal{P}_{n-1}$ $= w_j$

(5)

Order $> n$ for n -point Q.F. ?
possible?

Theorem 7.3.12. Maximal order of n -point quadrature rule

The maximal order of an n -point quadrature rule is $2n$.

Proof (indirect) : Assume $Q(p) = \int_a^b p(t) dt \quad \forall p \in \mathcal{P}_{2n}$

$$p(t) := \prod_{j=1}^n (t - c_j)^2 \geq 0 \Rightarrow \int_a^b p(t) dt > 0$$

$$p \in \mathcal{P}_{2n} \quad \text{but} \quad Q(p) = \sum_{j=1}^n w_j p(c_j) = 0 \quad \square$$

Example: 2-point rule of order 4

$$Q_n(p) = \int_a^b p(t) dt \quad \forall p \in \mathcal{P}_3 \Leftrightarrow Q_n(\{t \mapsto t^q\}) = \frac{1}{q+1} (b^{q+1} - a^{q+1}), \quad q = 0, 1, 2, 3.$$

Enough to check exactness for basis of \mathcal{P}_3

4 equations for weights w_j and nodes $c_j, j = 1, 2$ ($a = -1, b = 1$), cf. Rem. 7.3.6

non-linear system of equ.

$$\begin{aligned} \int_{-1}^1 1 dt &= 2 = 1w_1 + 1w_2, \quad \int_{-1}^1 t dt = 0 = c_1w_1 + c_2w_2 \\ \int_{-1}^1 t^2 dt &= \frac{2}{3} = c_1^2 w_1 + c_2^2 w_2, \quad \int_{-1}^1 t^3 dt = 0 = c_1^3 w_1 + c_2^3 w_2. \end{aligned} \quad (7.3.14)$$

> weights & nodes: $\{w_2 = 1, w_1 = 1, c_1 = 1/3\sqrt{3}, c_2 = -1/3\sqrt{3}\}$

► quadrature formula (order 4): $\int_{-1}^1 f(x) dx \approx f\left(\frac{1}{\sqrt{3}}\right) + f\left(-\frac{1}{\sqrt{3}}\right)$ (7.3.15)

Optimist's assumption: \exists family of n -point quadrature formulas on $[-1, 1]$

$$Q_n(f) := \sum_{j=1}^n w_j^n f(c_j^n) \approx \int_{-1}^1 f(t) dt, \quad w_j \in \mathbb{R}, n \in \mathbb{N},$$

of order $2n \Leftrightarrow$ exact for polynomials $\in \mathcal{P}_{2n-1}$. (7.3.17)

Define $\bar{P}_n(t) := (t - c_1^n) \cdots (t - c_n^n), \quad t \in \mathbb{R} \Rightarrow \bar{P}_n \in \mathcal{P}_n. \quad \bar{P}_n(c_j^n) = 0$

$$q \in \mathcal{P}_{n-1} : \underbrace{\int_{-1}^1 q \bar{P}_n dt}_{\in \mathcal{P}_{2n-1}} = \sum_{j=1}^n w_j (q \bar{P}_n)(c_j) = 0$$

\uparrow leading coeff = 1
 \uparrow order $2n$

" $\bar{P}_n \perp \mathcal{P}_{n-1}$ " w.r.t. inner product $(f, g) \rightarrow \int_{-1}^1 (fg)(t) dt$

\bar{P}_n is defined by n coefficients

$$\int_{-1}^1 q \bar{P}_n dt = 0 \quad \forall q \in \mathcal{P}_{n-1} \Rightarrow n = \dim \mathcal{P}_{n-1} \text{ conditions}$$

$\Rightarrow \bar{P}_n \in \mathcal{P}_n$ unique

The nodes of an n -point quadrature formula, if it exists, must coincide with the zeros of the polynomial \bar{P}_n defined recursively by (7.3.20). of order $2n$

6

Theorem 7.3.21. Existence of n -point quadrature formulas of order $2n$

Let $\{\bar{P}_n\}_{n \in \mathbb{N}_0}$ be a family of non-zero polynomials that satisfies

- $\bar{P}_n \in \mathcal{P}_n$,
- $\int_{-1}^1 q(t) \bar{P}_n(t) dt = 0$ for all $q \in \mathcal{P}_{n-1}$ ($L^2([-1, 1])$ -orthogonality),
- The set $\{c_j^n\}_{j=1}^m$, $m \leq n$, of real zeros of \bar{P}_n is contained in $[-1, 1]$.

Then the quadrature rule (\rightarrow Def. 7.1.1) $Q_n(f) := \sum_{j=1}^m w_j^n f(c_j^n)$

with weights chosen according to Thm. 7.3.5 provides a quadrature formula of order $2n$ on $[-1, 1]$.

Proof: $p \in \mathcal{P}_{2n-1} : p = h \bar{P}_n + r$, $h, r \in \mathcal{P}_{n-1}$

["Polynomial division"]

$$\int_{-1}^1 p(t) dt = \int_{-1}^1 h(t) \bar{P}_n(t) dt + \int_{-1}^1 r(t) dt =$$

$$= \sum_{j=1}^m w_j^n (r(c_j^n) + h \bar{P}_n(c_j^n))$$

$$= p(c_j^n)$$

$$= Q_n(p)$$

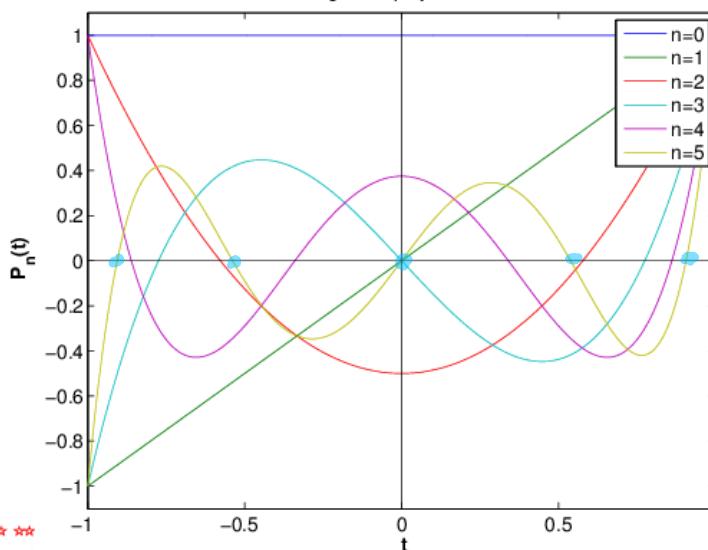
□

The polynomials \bar{P}_n :

Definition 7.3.26. Legendre polynomials

The n -th Legendre polynomial P_n is defined by

- $P_n \in \mathcal{P}_n$,
- $\int_{-1}^1 P_n(t) q(t) dt = 0 \forall q \in \mathcal{P}_{n-1}$,
- $P_n(1) = 1$.



◇ Obviously:

Zeros of Legendre polynomials in $[-1, 1]$

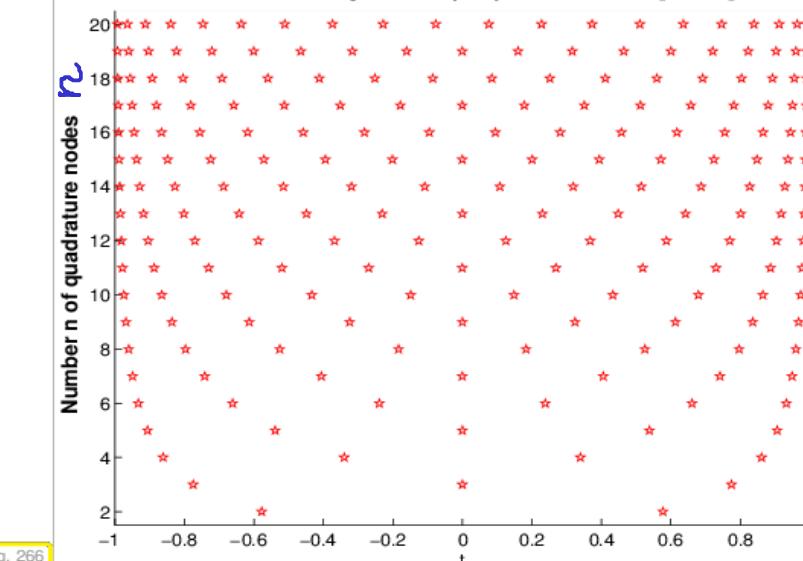


Fig. 266

Lemma 7.3.27. Zeros of Legendre polynomials

P_n has n distinct zeros in $[-1, 1]$.

Zeros of Legendre polynomials = Gauss points

nodes of unique n -pt Q.F. of order $2n$!

Proof: Assume : P_n has only $k < n$ zeros x_j in $J-1, 1E$

$$q(t) := \pm \prod_{j=1}^k (t - x_j) \Rightarrow P_n q \geq 0 \quad (*)$$

$$q \in \mathcal{P}_k$$

(*) Whenever P_n changes sign, also q changes sign.

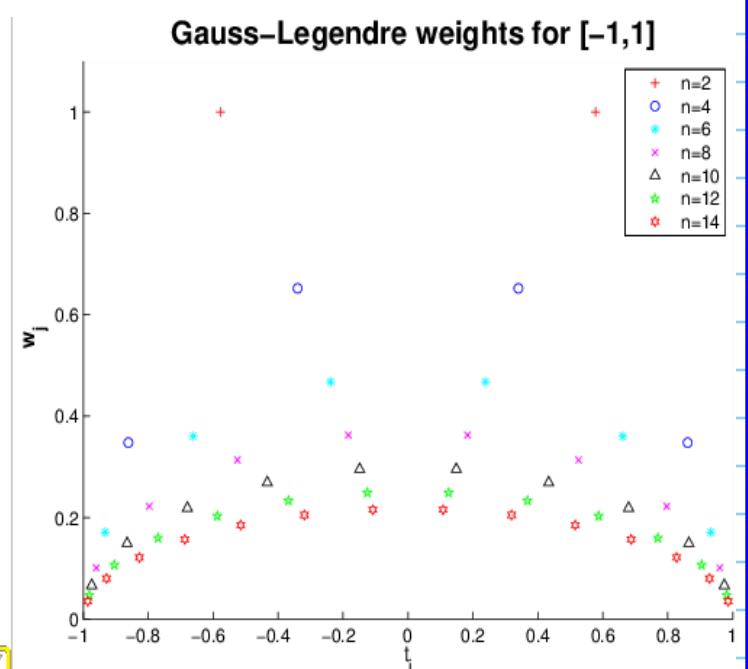
$$\int_{-1}^1 (P_n q)(t) dt \geq 0 \quad \square$$

(7)

Obviously

Lemma 7.3.30. Positivity of Gauss-Legendre quadrature weights

The weights of the Gauss-Legendre quadrature formulas are positive.



Proof: $\{t_j\}_{j=1}^n \stackrel{?}{=} \text{Gauss nodes}$,

$$q(t) := \prod_{\substack{j=1 \\ j \neq k}}^{n-1} (t - t_j)^2, \quad k \in \{1, \dots, n\}$$

$$q \in \mathcal{P}_{2n-2} : Q_n(q) = \sum_{j=1}^n w_j q(t_j) = \int q(t) dt$$

$\frac{\|q\|}{W_k (t_k - t_j)^2} > 0$

Order $2n$! \square

If Q.F. has order $q \geq 1 \Rightarrow Q_n(1) = \int_a^b 1 dt = b-a$

$$\frac{n}{\sum_{j=1}^n w_j} \cdot 1$$

- 1

Quadrature error \Leftrightarrow best approximation error

Q_n : Q.F. of order $q \geq 1 \Rightarrow E_n \stackrel{?}{=} \text{quadrature error}$

$$E_n(f) = E_n(f - p) \quad \forall p \in \mathcal{P}_{q-1}$$

$$f \in C^0([a, b]) = \left| \int_a^b (f - p)(t) dt - \sum_{j=1}^n w_j (f - p)(c_j) \right| \leq |b-a| \|f-p\|_{\infty, [a, b]} + \sum_{j=1}^n |w_j| \|f-p\|(c_j)$$

$$\leq \left(|b-a| + \sum_{j=1}^n |w_j| \right) \|f-p\|_{\infty}$$

$$\text{If } w_j \geq 0 \Rightarrow \sum_{j=1}^n |w_j| = b-a$$

$$\leq 2(b-a) \|f-p\|_{\infty} \quad \forall p \in \mathcal{P}_{q-1}$$

Theorem 7.3.39. Quadrature error estimate for quadrature rules with positive weights

For every n -point quadrature rule Q_n as in (7.1.2) of order $q \in \mathbb{N}$ with weights $w_j \geq 0, j = 1, \dots, n$ the quadrature error satisfies

$$E_n(f) := \left| \int_a^b f(t) dt - Q_n(f) \right| \leq 2|b-a| \inf_{\substack{p \in \mathcal{P}_{q-1} \\ \text{best approximation error}}} \|f-p\|_{L^\infty([a,b])} \quad \forall f \in C^0([a, b]). \quad (7.3.40)$$

\rightarrow applies to Gauss quadrature, Clenshaw-Curtis

⑧

Now apply polynomial best approximation estimates from Ch.

$$f \in C^r([a,b]), r \in \mathbb{N} \Rightarrow E_n(f) = O(n^{-r})$$

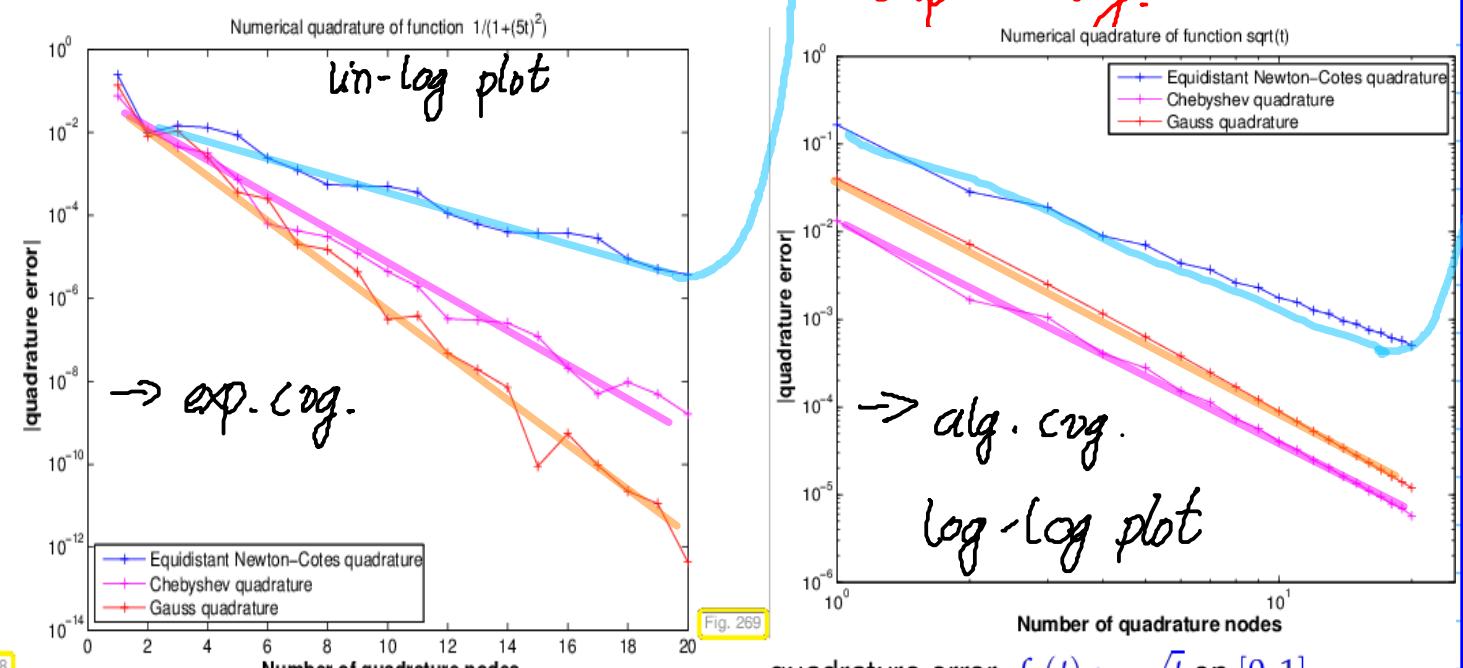
[if $q \geq r$]

\uparrow
order of Q.F.

$$f \in C^\infty([a,b]) \Rightarrow E_n(f) = O(q^n) \quad 0 \leq q < 1$$

for $n \rightarrow \infty$

\cong exp. cog.



$$\text{quadrature error, } f_1(t) := \frac{1}{1+(5t)^2} \text{ on } [0,1]$$

"Smoothing" integrands by transformation

$$\int_a^b \sqrt{t} f(t) dt \quad \text{with } f \in C^\infty([0,b])$$

\hookrightarrow non-smooth integrand : slow alg. cog. of quad. error

$$\text{Idea: substitution: } s = \sqrt{t} \Rightarrow \frac{ds}{dt} = \frac{1}{2\sqrt{t}} \Rightarrow dt = 2sds$$

$$\int_a^b \sqrt{t} f(t) dt = \int_0^{\sqrt{b}} s f(s^2) 2s ds$$

$$\in C^\infty([0, \sqrt{b}])!$$

\hookrightarrow exp. cog. of Gauss quadrature

Remark: How to read asymptotic estimates

$$E_n(f) = O(n^{-r})$$

for $n \rightarrow \infty$

$$E_n(f) \approx C n^{-r} \quad (*)$$

[assume ↑ sharp estimate]

Note: $C \geq 0$ unknown

(*) \Rightarrow no information for concrete n !

⑨

(*) tells us how much additional work
 $(=$ additional f-evaluations) is needed
to reduce the error by factor $S \geq 1$.

$$E_{n_{\text{old}}}(f) : E_{n_{\text{new}}}(f) = S$$

(*) \Rightarrow

$$\frac{n_{\text{old}}^{-r}}{n_{\text{new}}^{-r}} = S$$

$$n_{\text{new}} = n_{\text{old}} \cdot S^{\frac{1}{r}}$$

The larger r , the less the additional effort to gain a fixed error reduction!

5.4. Composite quadrature

\hookrightarrow Q.F. induced by p.w. polynomial interp.

Other perspective: On mesh $\mathcal{M} := \{a = x_0 < x_1 < \dots < x_m = b\}$

$$\int_a^b f(t) dt = \sum_{j=1}^m \int_{x_{j-1}}^{x_j} f(t) dt$$

apply n_j -pt local Q.F. on $[x_{j-1}, x_j]$

General construction of composite quadrature rules



Idea:

- Partition integration domain $[a, b]$ by a mesh/grid (\rightarrow Section 6.5)

$$\mathcal{M} := \{a = x_0 < x_1 < \dots < x_m = b\}$$

- Apply quadrature formulas from Section 7.2, Section 7.3 locally on mesh intervals $I_j := [x_{j-1}, x_j], j = 1, \dots, m$, and sum up.

composite quadrature rule

$$\# \text{f-eval} = \sum_{j=1}^m n_j$$

(1D)

Examples :

Composite trapezoidal rule, cf. (7.2.5)

$$\int_a^b f(t) dt = \frac{1}{2}(x_1 - x_0)f(a) + \sum_{j=1}^{m-1} \frac{1}{2}(x_{j+1} - x_{j-1})f(x_j) + \frac{1}{2}(x_m - x_{m-1})f(b).$$

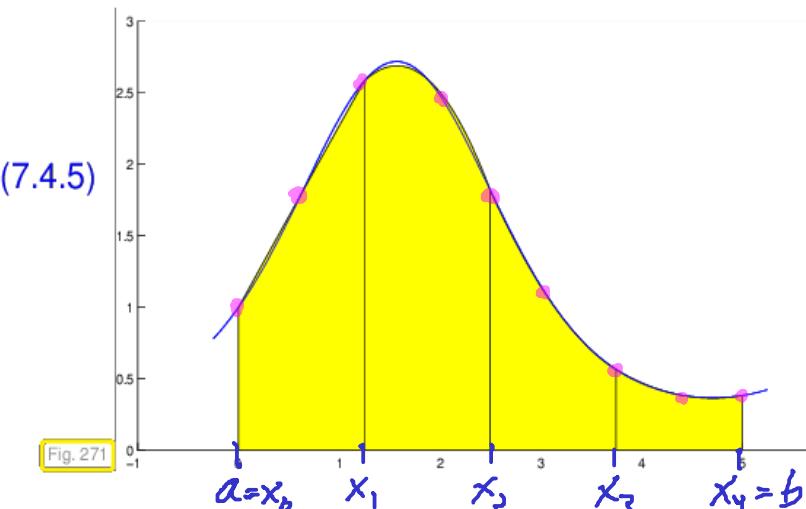
(7.4.4)

p.w. linear
interpolant

Composite Simpson rule, cf. (7.2.6)

$$\int_a^b f(t) dt = \frac{1}{6}(x_1 - x_0)f(a) + \sum_{j=1}^{m-1} \frac{1}{6}(x_{j+1} - x_{j-1})f(x_j) + \sum_{j=1}^m \frac{2}{3}(x_j - x_{j-1})f\left(\frac{1}{2}(x_j + x_{j-1})\right) + \frac{1}{6}(x_m - x_{m-1})f(b).$$

(7.4.5)



Error estimates for comp. quad. by summing local quadrature errors

For pol. local Q.F. of order q_j on $[x_{j-1}, x_j]$

$$\left| \int_{x_{j-1}}^{x_j} f(t) dt - Q_{n_j}^j(f) \right| \leq C |x_j - x_{j-1}|^{\min\{r, q_j\}+1} \|f^{(\min\{r, q_j\})}\|_{L^\infty([x_{j-1}, x_j])}. \quad (7.2.10)$$

independent of j for $f \in C^r([a, b])$

$$\sum_{(r \text{ big})} \Rightarrow E_n(f) \leq C \sum_{j=1}^m h_j^{q_j+1} \|f^{(q_j+1)}\|_{\infty, [x_{j-1}, x_j]}$$

(*) From polynomial error estimates for interpolation
 $(f - p)(t) = \frac{1}{(q+1)!} f^{(q+1)}(\xi) \prod_{j=0}^q (t - t_j)$

Now assume : $q = q_j \forall j$

$$E_n(f) \leq C h_m^q \|f^{(q+1)}\|_{\infty, [a, b]} \underbrace{\sum_j h_j}_{= b - a}$$

$$h_m = \max_j h_j$$

$$\left| \int_{x_0}^{x_m} f(t) dt - Q(f) \right| \leq C h_M^{\min\{q,r\}} |b-a| \|f^{(\min\{q,r\})}\|_{L^\infty([a,b])}, \quad (7.4.10)$$

fixed $q \Rightarrow$ [↑] alg. conv. in meshwidth h_M *

for f big (\Leftrightarrow smooth f) : rate = q [= order of local Q.F.]

* also called h -convergence

[reduction of quadrature error by using finer and finer meshes]

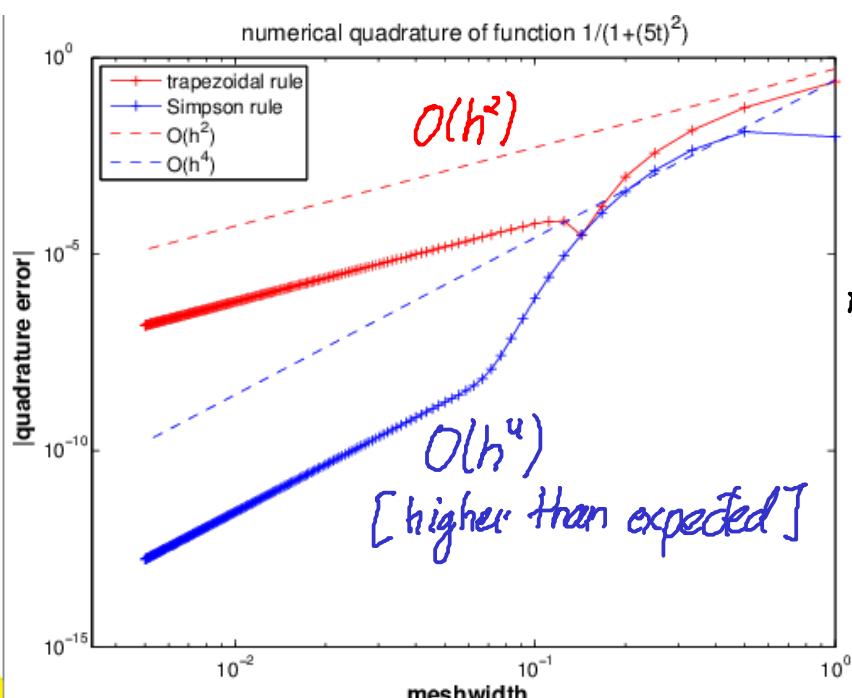


Fig. 272

quadrature error, $f_1(t) := \frac{1}{1+(5t)^2}$ on $[0, 1]$

(local order q)

Comparison : Comp. Quad. \Leftrightarrow Gauss quad.

$f \in C^r([a,b]) :$ $O(n^{-\min\{r,q\}})$ \downarrow $O(n^{-r})$

G.Q. is at least as good as comp. quad.

\rightarrow achieves best possible rate

$f \in C^\infty([a,b]) :$ $O(n^{-q})$ $O(q^n)$

with $0 \leq q < 1$

much faster

< equidistant mesh

log-log plot
"Linear" error graphs
 \approx alg. conv.