Numerical Methods for Computational Science and Engineering

Fall Semester 2017 (HS17)

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Obviously ▷

Lemma 7.3.30. Positivity of Gauss-Legendre quadrature weights

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

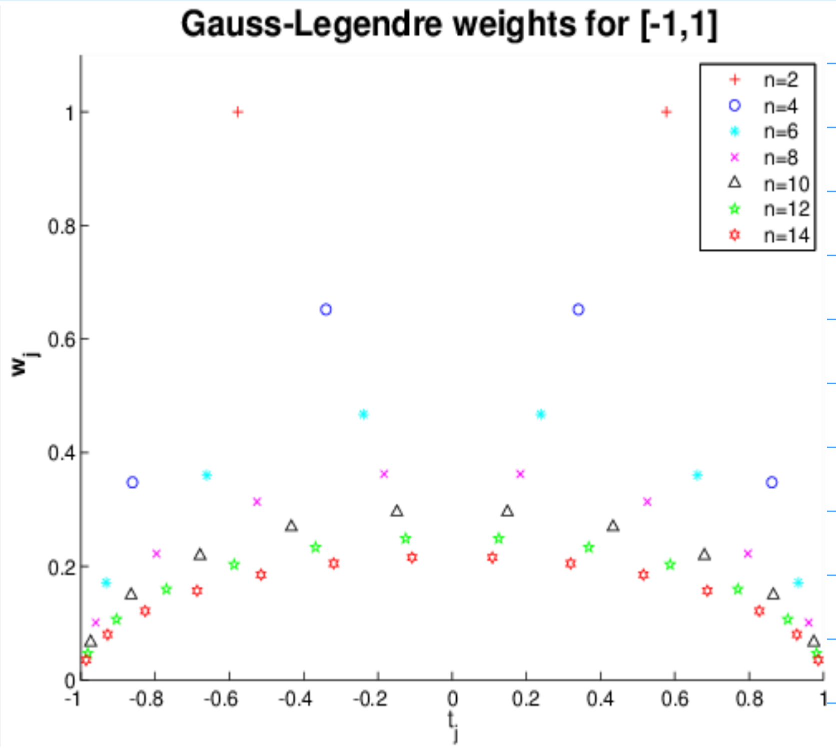

Fig. 267

Proof: Let ξ_j^n, $j=1,\dots,n$ denote Gauss points of n-point Gauss-Legendre QF.

1

Define $q_k(t) := \prod_{\substack{j=1 \\ j\neq k}}^{n} (t-\xi_j^n)^2$

$\Rightarrow q_k \in \mathcal{P}_{2n-2}$

$$\Rightarrow 0 < \int_{-1}^{1} q_k(t)\,dt = \sum_{j=1}^{n} w_j^n \cdot q_k(\xi_j^n)$$

order of n-point G.-L. QF: $2n$

$$= w_k^n \cdot \underbrace{q_k(\xi_k^n)}_{>0}$$

$q_k(\xi_j^n)=0 \;\; \forall j\neq k$

$\Rightarrow w_k^n > 0$ for $k=1,\dots,n$. □

Legendre polynomials satisfy 3-term recursion (similar to Chebychev polynomials)

$$P_{n+1}(t) := \frac{2n+1}{n+1} t P_n(t) - \frac{n}{n+1} P_{n-1}(t) \quad , \quad P_0 := 1 \, , \quad P_1(t) := t \, . \qquad (7.3.33)$$

Note: Chebychev polynomials are also family of L^2-orth. polynomials (but w.r.t. weighted L^2-norm)

Quadrature error & best approximation error

Use positivity of weights to obtain:

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 $w_j \geq 0$, $j = 1, \ldots, n$ the quadrature error satisfies

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

Proof: $E_n(f) \underset{p \in \mathcal{P}_{q-1}}{\overset{\uparrow}{=}} E_n(f-p) = \left| \int_a^b (f-p)(t)\,dt - \sum_{j=1}^n \omega_j (f-p)(c_j) \right|$

$$\leq \left| \int_a^b (f-p)(t)\,dt \right| + \left| \sum_{j=1}^n \omega_j \cdot (f-p)(c_j) \right|$$

$$\leq |b-a| \cdot \|f-p\|_{L^\infty([a,b])} + \underbrace{\left(\sum_{j=1}^n |\omega_j| \right)} \cdot \|f-p\|_{L^\infty([a,b])}$$

Positivity of ω_j implies:

$$\sum_j |\omega_j| = \sum_j \omega_j$$

for $q \geq 1$: $\quad Q_n(1) = \sum_j \omega_j \cdot 1 = \int_a^b 1 \cdot dt = b-a$

$$\Rightarrow \sum_j |\omega_j| = \sum_j \omega_j = b-a$$

$$E_n(f) \leq 2 \cdot |b-a| \cdot \underbrace{\inf_{p \in \mathcal{P}_{q-1}} \|f-p\|_{L^\infty([a,b])}} \qquad \square .$$

Asymptotic behavior $E_n(f)$ as $n \to \infty$.

Lemma 7.3.42. Quadrature error estimates for C^r-integrands

For every n-point quadrature rule Q_n as in (7.1.2) of order $q \in \mathbb{N}$ with weights $w_j \geq 0$, $j = 1, \ldots, n$ we find that the quadrature error $E_n(f)$ for and integrand $f \in C^r([a,b])$, $r \in \mathbb{N}_0$, satisfies

$$\text{in the case } q \geq r: \quad E_n(f) \leq C q^{-r} |b-a|^{r+1} \left\| f^{(r)} \right\|_{L^\infty([a,b])}, \tag{7.3.43}$$

$$\text{in the case } q < r: \quad E_n(f) \leq \frac{|b-a|^{q+1}}{q!} \left\| f^{(q)} \right\|_{L^\infty([a,b])}, \tag{7.3.44}$$

with a constant $C > 0$ independent of n, f, and $[a,b]$.

If $f \in C^r([a,b])$: algebraic convergence with rate $\underline{\underline{r}}$

$f \in C^\infty([a,b])$: exponential convergence.

1. $f_1(t) = \frac{1}{1+(5t)^2}$, an analytic function, see Rem. 6.1.72,
2. $f_2(t) = \sqrt{t}$, merely continuous, derivatives singular in $t = 0$.

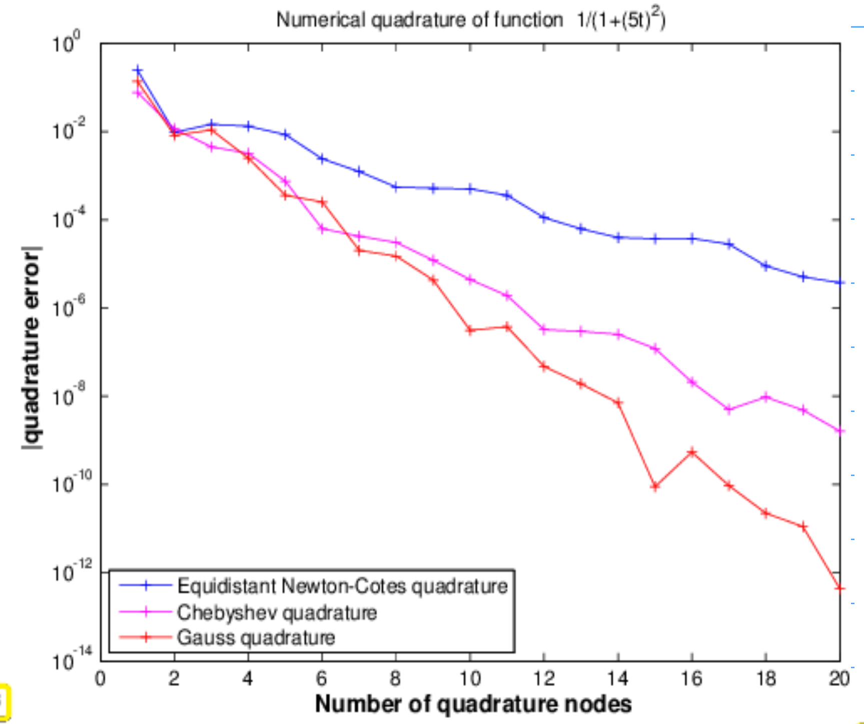

Fig. 268

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

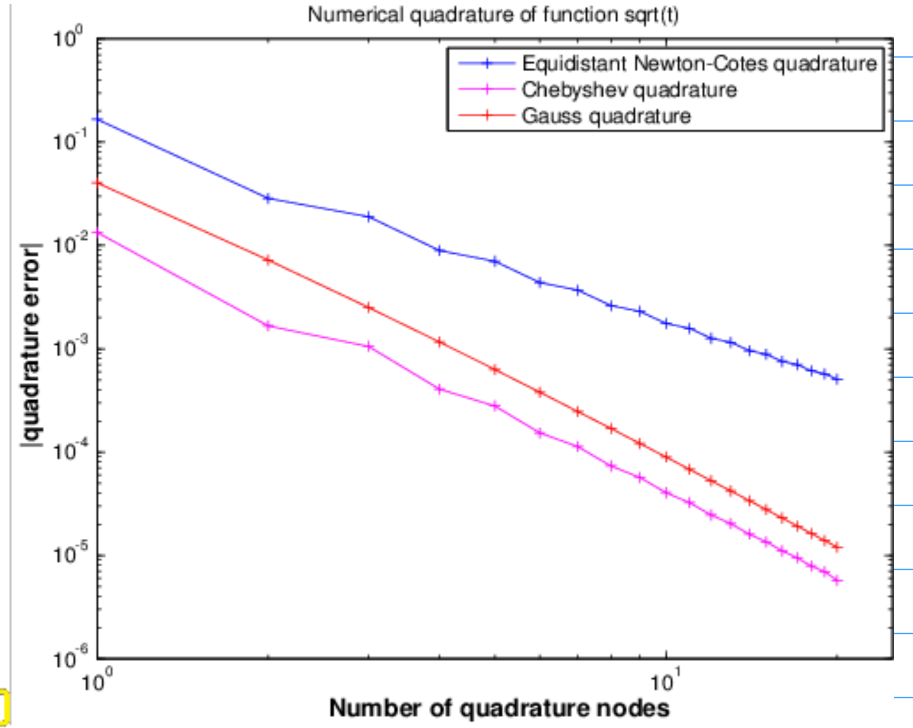

Fig. 269

quadrature error, $f_2(t) := \sqrt{t}$ on $[0,1]$

lin-log-plot

exponential conv.

log-log-plot

algebraic conv.

Note: Error of equidistant QF blows up as number of nodes increases

Remark on Example 2: $f(t)=\sqrt{t}$ $t=[0,1]$

Task: Approximate $\int_0^1 \sqrt{t}\, dt$

Substitution: $s=\sqrt{t}$

$$dt = 2s\, ds$$

$$\int_0^1 s \cdot 2s\, ds = \underbrace{\int_0^1 \underbrace{2s^2}_{\in C^\infty} ds}_{\text{apply QF here}}$$

More generally:

Approximate $\int_0^b \sqrt{t}\, g(t)\, dt$ $g \in C^\infty([0,b])$

Substitute $s=\sqrt{t}$

$$\Rightarrow \int_0^b \sqrt{t}\, g(t)\, dt = \int_0^{\sqrt{b}} \overbrace{2s^2\, g(s^2)}^{\in C^\infty([0,b])} ds$$

Remark: What does the asymptotic behavior really tell us?

[Since there are "hidden constants" in such estimates]

Example 1: Fix integrand f and assume sharp algebraic convergence for family of n-point QFs

$$E_n(f) = \Theta(n^{-r}) \xrightarrow{\text{sharpness}} E_n(f) \approx C \cdot n^{-r}$$

$C>0$ indep. of n

Task: Change QF to reduce quadrature error by factor $\rho > 1$.

i.e. minimal increase in number n of quadrature points.

$$\frac{C \cdot n_{old}^{-r}}{C \cdot n_{new}^{-r}} \overset{!}{=} \rho \iff \boxed{n_{new} = n_{old} \cdot \rho^{1/r}}$$

Asymptotics tell us: increase number of points by factor $\rho^{1/r}$

Note: Improving in accuracy is cheaper for larger r [i.e. smoother integrand]

Example 2: Sharp exp. convergence of family of n-point QF (for a fixed integrand f)

$$E_n(f) = \Theta(\underset{\substack{\uparrow \\ \in (0,1)}}{\lambda}^n) \Rightarrow E_n(f) \approx \underset{\substack{\uparrow \\ \text{ind. of } n}}{C} \cdot \lambda^n$$

Reduce error by factor $\rho > 1$:

$$\frac{C \cdot \lambda^{n_{old}}}{C \cdot \lambda^{n_{new}}} \overset{!}{=} \rho \iff \lambda^{n_{old} - n_{new}} = \rho$$

$$\iff (n_{old} - n_{new}) \cdot \log \lambda = \log \rho$$

$$n_{new} - n_{old} = \underbrace{-\frac{\log \rho}{\log \lambda}}_{>0}$$

$$n_{new} = n_{old} + \left\lceil \left| \frac{\log \rho}{\log \lambda} \right| \right\rceil$$

$\Rightarrow$ To reduce error by a factor ρ always add a fixed number of points $\left\lceil \left| \frac{\log \rho}{\log \lambda} \right| \right\rceil$.

7.4. Composite Quadrature

As done for interpolation:

Divide interval with a mesh and apply a QF on each cell.

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

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

on each $I_j = [x_{j-1}, x_j]$: apply n_j-point QF.

number of f evaluations: $\sum_{j=1}^{m} n_j$

<u>"Composite QF"</u>

Examples:

Composite trapezoidal rule, *cf.* (7.2.5)

$$\int_a^b f(t)\mathrm{d}t = \tfrac{1}{2}(x_1 - x_0)f(a) + \sum_{j=1}^{m-1} \tfrac{1}{2}(x_{j+1} - x_{j-1})f(x_j) + \tfrac{1}{2}(x_m - x_{m-1})f(b)\,. \tag{7.4.4}$$

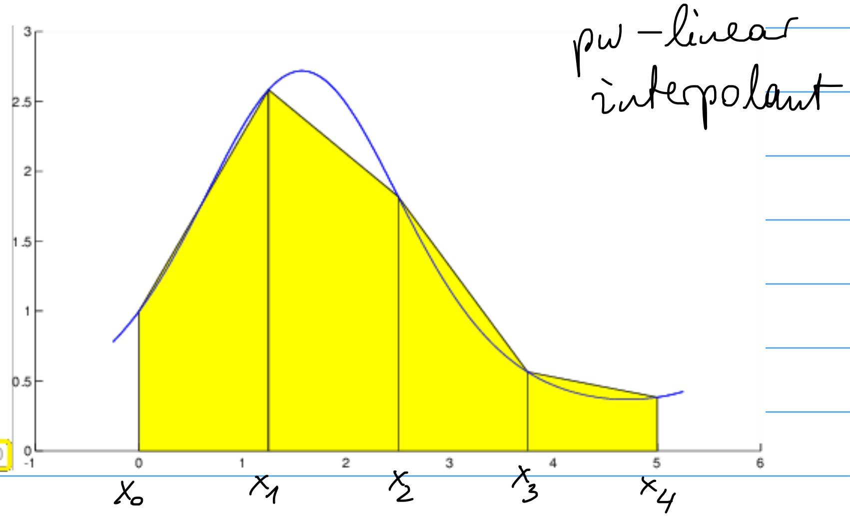

Fig. 270

Composite Simpson rule, *cf.* (7.2.6)

$$\int_a^b f(t)\mathrm{d}t = \tfrac{1}{6}(x_1 - x_0)f(a) + \sum_{j=1}^{m-1} \tfrac{1}{6}(x_{j+1} - x_{j-1})f(x_j) + \sum_{j=1}^{m} \tfrac{2}{3}(x_j - x_{j-1})\underline{f(\tfrac{1}{2}(x_j + x_{j-1}))} + \tfrac{1}{6}(x_m - x_{m-1})f(b)\,. \tag{7.4.5}$$

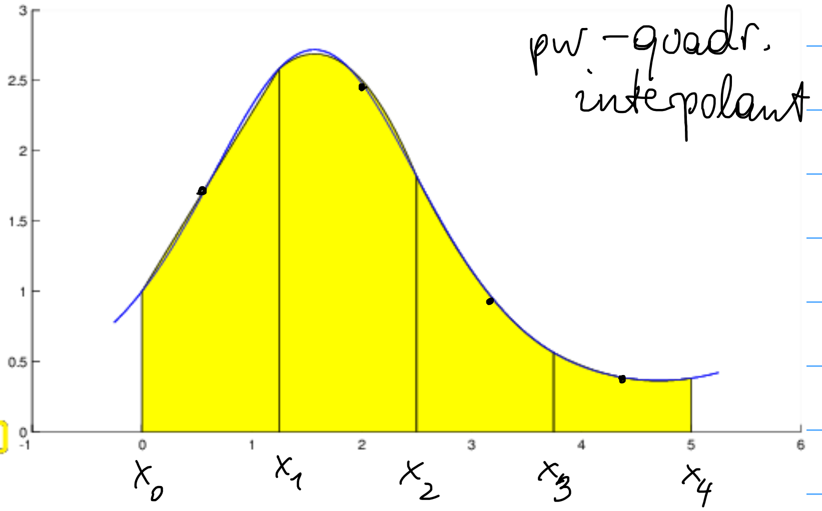

Fig. 271

Error estimates for composite QF?

$\rightsquigarrow$ add errors on each I_j

Suppose on each I_j: QF $Q^j_{n_j}$ of order q_j

and with positive weights

For $f \in C^r([x_{j-1}, x_j])$ we have:

$$\left| \int_{x_{j-1}}^{x_j} f(t)\,dt - Q^j_{n_j}(f|_{I_j}) \right| \leq C \cdot h_j^{\min\{r,q_j\}+1} \cdot \| f^{(\min\{r,q\})} \|_{L^\infty(I_j)}$$

ind. of j $\quad$ $h_j = |x_j - x_{j-1}|$

$$\Rightarrow \left| \sum_{j=1}^m \left\{ \int_{x_{j-1}}^{x_j} f(t)\,dt - Q^j_{n_j}(f) \right\} \right| \leq \sum_{j=1}^m \left| \int_{x_{j-1}}^{x_j} f(t)\,dt - Q^j_{n_j}(f) \right|$$

$$\leq C \cdot \sum_{j=1}^m h_j^{\min\{r,q_j\}+1} \cdot \| f^{(\min\{r,q\})} \|_{L^\infty(I_j)} \qquad (*)$$

Define $h_\mu = \max h_j$ for $q_j = q$

$$(*) \leq C \cdot h_\mu^{\min\{r,q\}} \cdot \max_{j=1,\dots,m} \| f^{(\min\{r,q\})} \|_{L^\infty(I_j)} \cdot \underbrace{\sum_{j=1}^m h_j}_{|b-a|}$$

$$\leq C \cdot h_\mu^{\min\{r,q\}} \cdot |b-a| \cdot \max_{j=1,\dots,m} \| f^{(\min\{r,q\})} \|_{L^\infty(I_j)}$$

algebraic convergence in h_μ (mesh width)

"h-convergence"

for r large (f is smooth): algebraic convergence in h_μ of rate q.

Example: Composite QF on equidistant mesh for smooth vs non-smooth function

Composite trapezoidal: $q = 2$

Simpson: $q = 4$ (more than expected)

For smooth functions: $\mathcal{O}(h^2)$ vs. $\mathcal{O}(h^4)$

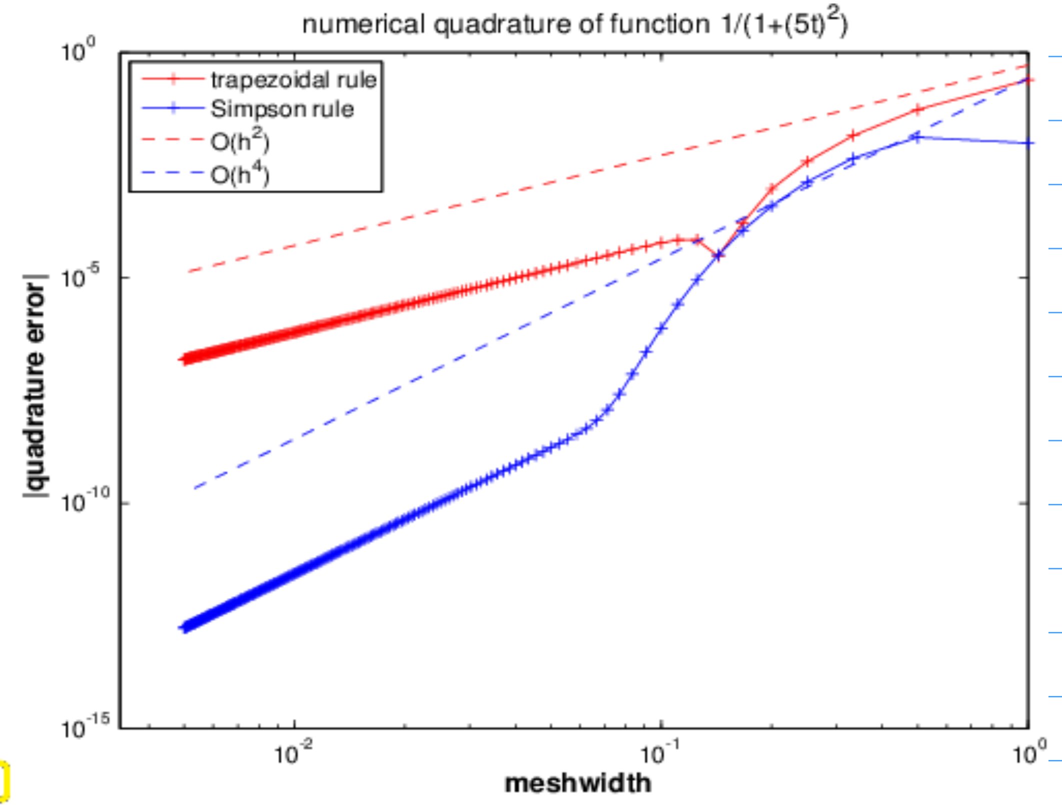

Fig. 272

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

log-log-plot

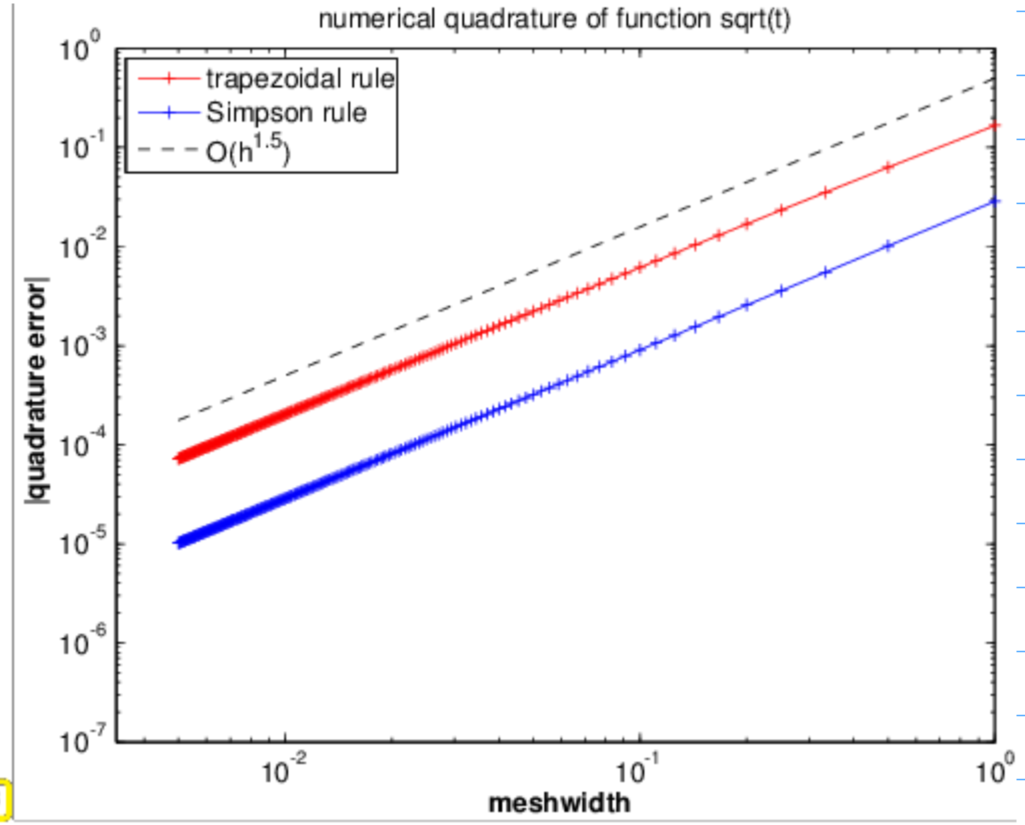

Fig. 273

quadrature error, $f_2(t) := \sqrt{t}$ on $[0,1]$

$\mathcal{O}(h^{3/2})$ (note: f_2 not smooth at $t=0$)

Remark: Comparison of asymptotic rates of composite QFs vs global Gauss QF:

$f \in C^r([a,b])$: composite QF (with local order q): $\Theta(n^{-\min\{r,q\}})$

Gauss QF : $\Theta(n^{-r})$

$\Rightarrow$ Gauss at least as good as composite QF and achieves best-possible rate

$f \in C^\infty([a,b])$: composite QF : $\Theta(n^{-q})$ alg. conv.

Gauss QF : $\Theta(\lambda^n)$ exp. conv.

$\lambda \in (0,1)$