

# Numerical Methods for Computational Science and Engineering

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Numerical integration on arbitrary intervals  $[a, b]$

$\leadsto$  we can reduce this to finding QF on  
a reference interval, e.g.  $[-1, 1]$

Suppose: We know a QF:  $(\hat{c}_j, \hat{w}_j)_{j=1}^n$  on  $[-1, 1]$

$$\left[ \text{QF}(f) = \sum_{j=1}^n \hat{w}_j f(\hat{c}_j) \right]$$

We want QF on  $[a, b]$ :

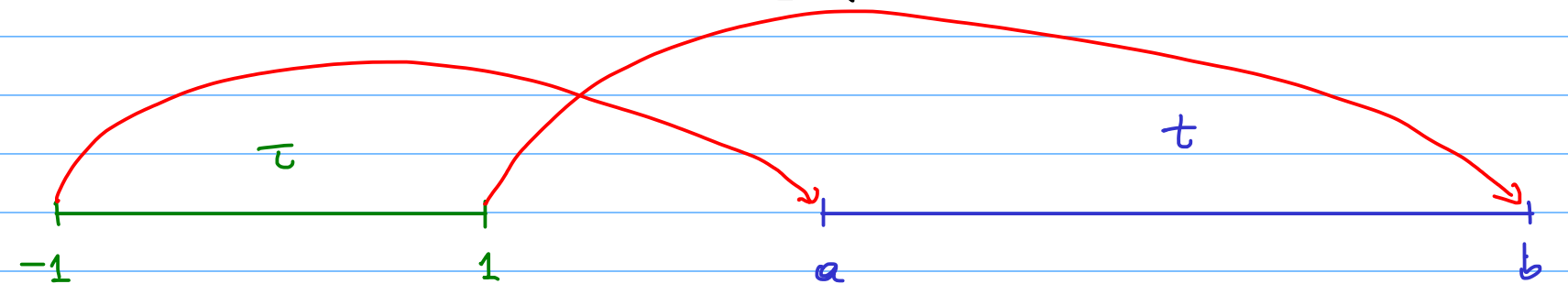
$$\text{Approximate } \int_a^b f(t) dt !$$

↓

can be transformed to  $[-1, 1]$ :

$$\int_a^b f(t) dt = \int_{-1}^1 f(\bar{\Phi}(\tau)) \bar{\Phi}'(\tau) d\tau$$

$$\bar{\Phi}(\tau) = \frac{1}{2}(1-\tau)a + \frac{1}{2}(1+\tau)b$$



$$\int_a^b f(t) dt \approx \frac{1}{2} (b-a) \sum_{j=1}^n \hat{\omega}_j \hat{f}(\hat{c}_j)$$

$$= \sum_{j=1}^n \omega_j f(c_j) \quad (\hat{f} = f \circ \Phi)$$

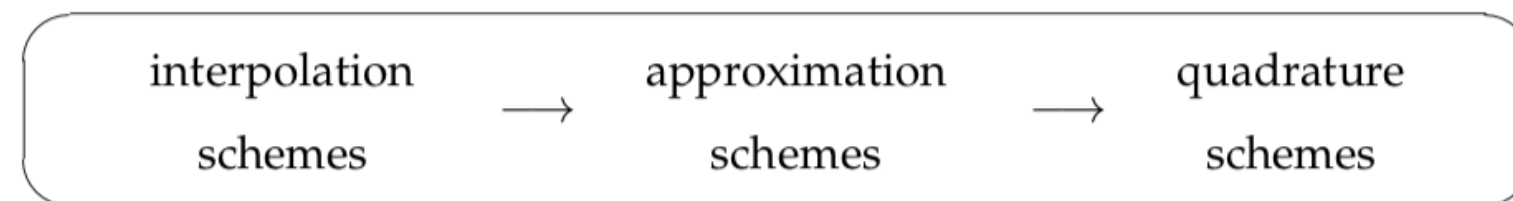
$$c_j = \frac{1}{2} (1 - \hat{c}_j) a + \frac{1}{2} (1 + \hat{c}_j) b$$

$$\omega_j = \frac{1}{2} (b-a) \hat{\omega}_j$$

$$(c_j, \omega_j) \quad \text{QF for } [a, b]$$

$$(\hat{c}_j, \hat{\omega}_j) \quad \text{QF for } [-1, 1]$$

## Quadrature by approximation schemes



Suppose we have an approximation scheme

$$A: C^0([a, b]) \rightarrow V$$

↑  
space of "simple" functions

Then, we want to perform numerical integration as:

$$\int_a^b f(t) dt \approx \int_a^b (Af)(t) dt =: Q_A(f)$$

Use interpolation schemes:

$$I_{\mathcal{T}}(f) \quad \mathcal{T} = \{t_1, \dots, t_n\} \text{ node set}$$

↑  
interpolation of  $f(t_1), \dots, f(t_n)$

$$\int_a^b f(t) dt \quad \text{instead:}$$
$$\approx \int_a^b I_{\mathcal{T}}[f(t_1), \dots, f(t_n)]^T(t) dt$$

For this to work, the interpolation operator needs to be linear.

$$\int_a^b I_{\mathcal{T}}[f(t_1), \dots, f(t_n)]^T(t) dt$$
$$= \int_a^b I_{\mathcal{T}}\left[\sum_{i=1}^n f(t_i) e_i\right]^T(t) dt$$

$$[f(t_1), \dots, f(t_n)] = \sum_{i=1}^n f(t_i) e_i$$

$$= \sum_{i=1}^n f(t_i) \underbrace{\int_a^b I_{\mathcal{T}}[e_i](t) dt}_{=: w_i} = \sum_{i=1}^n f(t_i) w_i$$

linearity  
of  $I_{\mathcal{T}}$

↑  
this is a QF

Quality of the interpolation gives a bound  
on the error of the QF

$$E_n(f) = \left| \int_a^b (f(t) - I_{\mathcal{T}}[f(t_1), \dots, f(t_n)]^T(t)) dt \right|$$

$$\leq |b-a| \cdot \underbrace{\|f - I_{\mathcal{T}}[f(t_1), \dots, f(t_n)]^T\|_{L^\infty([a,b])}}_{\text{interpolation error}}$$

## Polynomial QFs

Idea:

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

$p_{n-1}$  polynomial Lagrange interpolant  
of  $f$  for a given node set  
 $\mathcal{T} := \{t_0, \dots, t_{n-1}\} \subset [a, b]$

$$p_{n-1}(t) = \sum_{i=0}^{n-1} f(t_i) \cdot L_i(t)$$

Recall Lagrange polyn.  $L_i(t) = \prod_{\substack{j=0 \\ j \neq i}}^{n-1} \frac{t - t_j}{t_i - t_j}$

$$QF: \int_a^b P_{n-1}(t) dt = \int_a^b \left( \sum_{i=0}^{n-1} f(t_i) L_i(t) \right) dt$$

$$= \sum_{i=0}^{n-1} f(t_i) \cdot \int_a^b L_i(t) dt$$

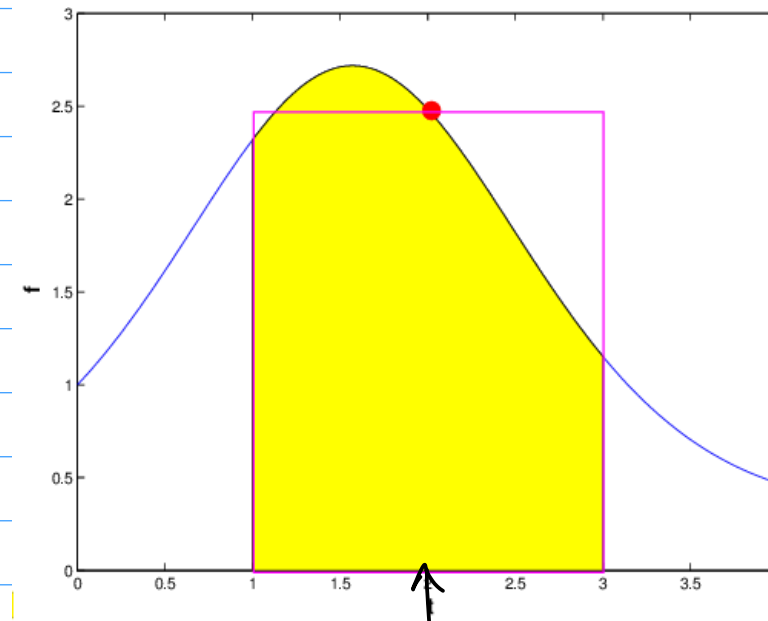
$$= \sum_{i=1}^n f(t_{i-1}) \int_a^b L_{i-1}(t) dt$$

weights:  $w_i := \int_a^b L_{i-1}(t) dt$

$$c_i := t_{i-1}$$

Examples:

$n=1$  midpoint rule



$$t_0 = \frac{1}{2}(a+b)$$

Approximation of  $f$  by  
a constant polynomial

$$Q_{mp}(f) = (b-a) \cdot f(t_0)$$

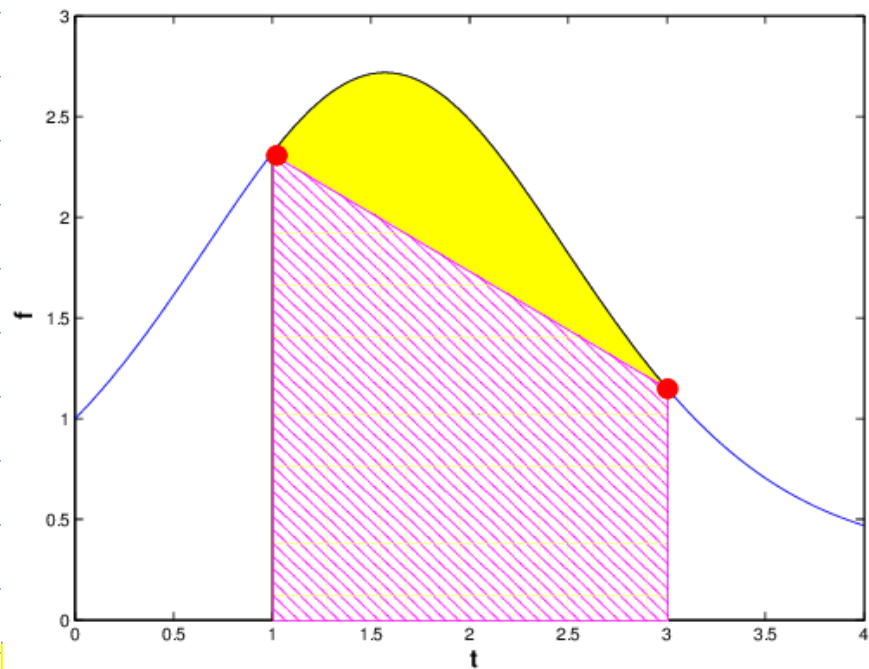
More generally: Newton-Cotes formulas  
 $n$ -point Newton-Cotes formula

Equidistant nodes & Lagrange interpolation



$$t_j := a + \frac{b-a}{n-1} j \quad j=0, \dots, n-1$$

$n=2$  trapezoidal rule



Approximation of  $\int_a^b f(t) dt$  by a linear polynomial

$$Q_{tr}(f) = \frac{b-a}{2} (f(a) + f(b))$$
$$= w_1 f(a) + w_2 f(b)$$

$$w_i = \int_a^b L_{i-1}(t) dt$$

$$w_1 = \int_a^b L_0(t) dt = \int_a^b \frac{t-b}{a-b} dt = \frac{b-a}{2}$$

$$w_2 = \int_a^b L_1(t) dt = \int_a^b \frac{t-a}{b-a} dt = \frac{b-a}{2}$$

$n=3$  Simpson rule

$$\int_a^b f(t) dt \approx \frac{b-a}{6} \left( f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right)$$

Polynomial QF based on Lagrange interpolation is straight-forward

BUT: Lagrange interpolation with equidistant nodes is numerically unstable

Remedy: Use Chebyshev nodes instead  
→ yield Clenshaw-Curtis QF.

## Gauss Quadrature

↳ in some sense the optimal choice for polynomial QF and a given budget  $n$  of points.

This requires a concept of quality for QFs.

→ Order of a QF

**Definition 6.3.1** (Order of a quadrature rule). The order of quadrature rule  $Q_n : C^0([a, b]) \rightarrow \mathbb{R}$  is defined as

$$\text{order}(Q_n) := \max\{m \in \mathbb{N}_0 : Q_n(p) = \int_a^b p(t) dt \quad \forall p \in \mathcal{P}_m\} + 1, \quad (6.11)$$

that is, as the maximal degree +1 of polynomials for which the quadrature rule is guaranteed to be exact.

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

↑  
up to which degree is this exact for polynomials

Note: This concept of order of a QF  
is invariant under affine transformations  
(such as  $\Phi$  from before to transform  
from  $[-1, 1]$  to  $[a, b]$ ).

Example: Suppose we have a polynomial QF  
with  $n$  points.

What can we say about its order?

Polynomial QF with  $n$  points:

is based on polynomial interpolation with  
 $n$  nodes

So: any  $p \in \mathcal{P}_{n-1}$  is uniquely determined by

$n$  values  $p(t_1), \dots, p(t_n)$

$\Rightarrow$  interpolation gives  $p$ .

$\Rightarrow$  quadrature is exact for any  $p \in \mathcal{P}_{n-1}$

This means  $\text{order}(\text{QF}_{\text{poly}}) \geq (n-1) + 1 = n$

[In fact, we will see that  $> n$  is possible]



Characterization of n-point QFs with order  $\geq n$ :

**Theorem 6.3.1** (Sufficient order conditions for quadrature rules). An n-point quadrature rule on  $[a, b]$  (see Definition 6.1.1)

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

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 (5.14) associated with the ordered node set  $\{t_1, t_2, \dots, t_n\}$ .

$$L_i(t) = \prod_{\substack{j=0 \\ j \neq i}}^{n-1} \frac{t - t_j}{t_i - t_j} \quad \leftarrow \text{determined by the nodes } t_0, \dots, t_{n-1}$$

Therefore: For QF  $Q_n$  to have order  $\geq n$   
weights  $w_j$  only depend on node set  
 $T = \{t_1, \dots, t_n\}$

Proof of Thm 6.3.1: Exercise

The big question: Are there n-point QFs with order  $> n$ ?

Upper bound to the order of an n-point QF:

**Theorem 6.3.2** (Maximal order of n-point quadrature rule). The maximal order of an n-point quadrature rule is  $2n$ .

Why? To see this, we construct a polynomial  $q \in \mathbb{P}_{2n}$  s.t.  $Q_n(q) \neq \int_a^b q(t) dt$ .

Because then: order  $< 2n+1$   
or  $\leq 2n$ .

How?

$$Q_n(f) := \sum_{j=1}^n w_j^n f(c_j^n)$$

with choice

$$q(t) := (t-c_1^n)^2 (t-c_2^n)^2 \cdots (t-c_n^n)^2 \in \mathbb{P}_{2n}$$
$$= t^{2n} + \dots$$

$$q(t) \geq 0 \quad (\text{by definition})$$

$$\Rightarrow \int_a^b q(t) dt > 0$$

On the other hand:

$$Q_n(q) = \sum_{j=1}^n w_j^n q(c_j^n) = 0$$

$$\Rightarrow Q_n(q) \neq \int_a^b q(t) dt$$

$$\Rightarrow \text{order}(Q_n) < 2n+1$$

$$\Rightarrow \text{order}(Q_n) \leq 2n \quad \square$$

Example: 2-point QF  $Q_2$  of order 4 on  $[-1, 1]$

$$Q_2(p) = \int_a^b p(t) dt \quad \forall p \in \mathbb{P}_3$$

$$\Leftrightarrow Q_2(\{t \mapsto t^q\}) = \frac{1}{q+1} (b^{q+1} - a^{q+1})$$

$$q = 0, 1, 2, 3$$

This is sufficient because monomials  $(\{t \mapsto t^q\})_{q=0}^n$  form a basis of  $\mathcal{P}_n$ .

$a = -1, b = 1$ :

$$\text{QF: } \int_{-1}^1 f(t) dt \approx \omega_1 f(c_1) + \omega_2 f(c_2)$$

$$\int_{-1}^1 1 dt = 2 \stackrel{\text{QF}}{=} \omega_1 + \omega_2 \quad (1)$$

$$\int_{-1}^1 t dt = \left. \frac{t^2}{2} \right|_{-1}^1 = \frac{1}{2} - \frac{1}{2} = 0 = \omega_1 c_1 + \omega_2 c_2 \quad (2)$$

$$\int_{-1}^1 t^2 dt = \left. \frac{t^3}{3} \right|_{-1}^1 = \frac{2}{3} = \omega_1 c_1^2 + \omega_2 c_2^2 \quad (3)$$

$$\int_{-1}^1 t^3 dt = 0 = \omega_1 c_1^3 + \omega_2 c_2^3 \quad (4)$$

Simple check:  $c_1, c_2, \omega_1, \omega_2$  are all  $\neq 0$

$$(2) \Rightarrow \omega_1 = -\frac{c_2}{c_1} \omega_2$$

$$(4) \Rightarrow \omega_1 = -\frac{c_2^3}{c_1^3} \omega_2$$

$$\Rightarrow \frac{c_2}{c_1} = \frac{c_2^3}{c_1^3} \Rightarrow \frac{c_2^2}{c_1^2} = 1$$

$$\Rightarrow c_1^2 = c_2^2$$

Use this in (3):

$$\frac{2}{3} = c_1^2 (\underbrace{\omega_1 + \omega_2}_{=2})$$

$\uparrow$   
(1)

$$\Rightarrow c_1^2 = \frac{1}{3}, \quad c_2^2 = \frac{1}{3}$$

Choose  $c_1, c_2$  s.t.  $c_1 \neq c_2 \Rightarrow c_1 = -c_2$

(2):  $\omega_1 c_1 + \omega_2 c_2 = 0$

$\omega_1 - \omega_2 = 0$

$\Rightarrow \underline{\omega_1 = \omega_2}$

Pick  $\underline{c_1 = -\frac{1}{\sqrt{3}}}, c_2 = \frac{1}{\sqrt{3}}$

(1):  $\omega_1 + \omega_2 = 2$

$\Rightarrow \underline{\omega_1 = 1}, \underline{\omega_2 = 1}$

$Q_2$ : 2-point QF of order 4:

$Q_2(f) = 1 \cdot f(-\frac{1}{\sqrt{3}}) + 1 \cdot f(\frac{1}{\sqrt{3}})$

More generally we can ask:

For any  $n \in \mathbb{N}$ , is there  $Q_n$  s.t.  
 $Q_n$  is  $n$ -point and  
of order  $2n$ ?

**Theorem 6.3.3** (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  $\{c_j^n\}_{j=1}^m, \underline{m \leq n}$ , of real zeros of  $\bar{P}_n$  is contained in  $[-1, 1]$ .

Then the quadrature rule (see Definition 6.1.1)  $Q_n(f) := \sum_{j=1}^m w_j^n f(c_j^n)$

with weights chosen according to Theorem 6.3.1 provides a quadrature formula of order  $2n$  on the interval  $[-1, 1]$ .

We will see:  $m = n$

$\bar{P}_n(t) = (t - c_1^n) \cdots (t - c_n^n)$

$n$ -point QF of order  $2n$

It turns out: Up to scaling factors, the  $\overline{P}_n$ 's are the Legendre polynomials

**Definition 6.3.2** (Legendre polynomials). The  $n$ -th Legendre polynomial  $P_n$  is defined by

- $P_n \in \mathcal{P}_n$ ,
- $\int_{-1}^1 P_n(t)q(t) dt = 0 \quad \forall q \in \mathcal{P}_{n-1}$ ,  $\langle P_n, q \rangle_{L^2([-1,1])} = 0$
- $P_n(1) = 1$ .

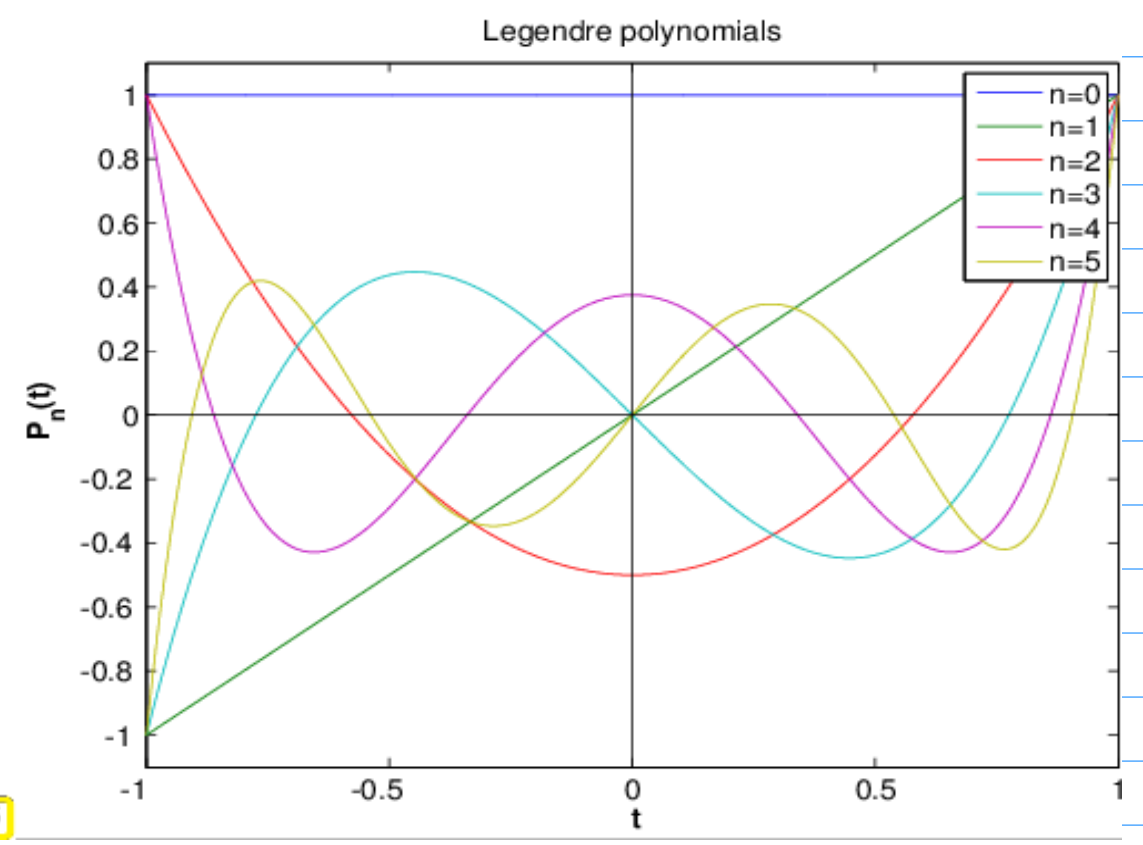


Fig. 265

Fact:  $P_n$  has  $n$  distinct zeros in  $(-1, 1)$

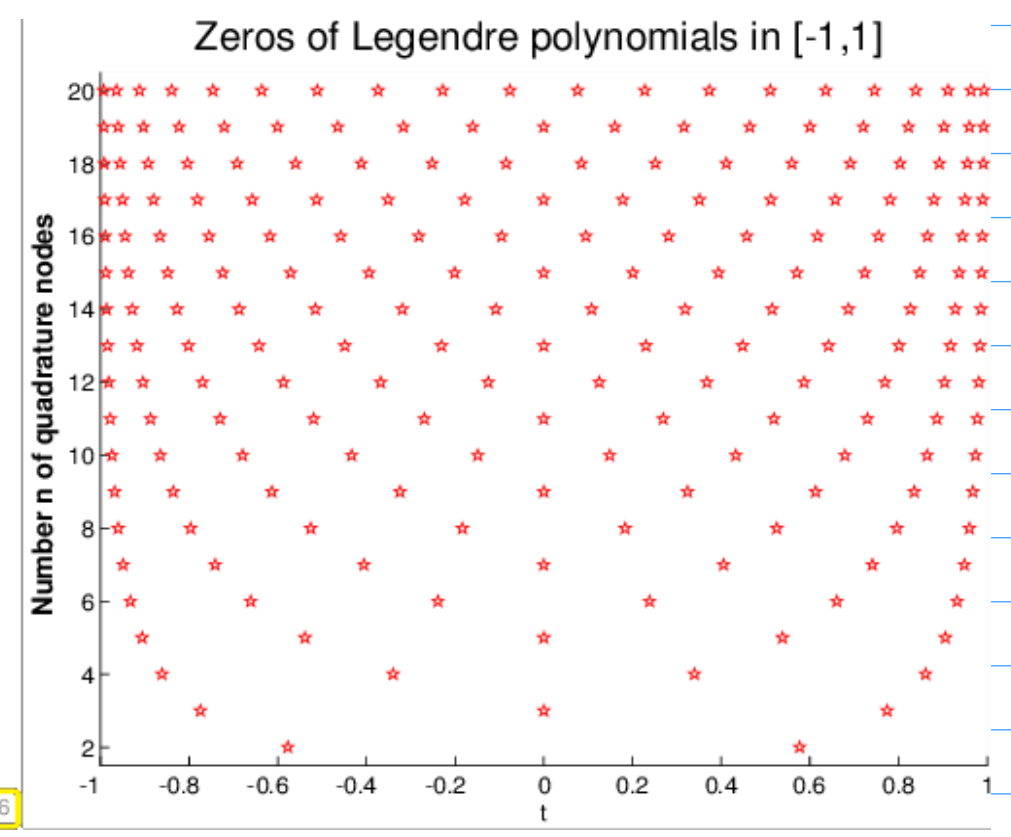


Fig. 266

Why does  $P_n$  have  $n$  distinct zeros in  $(-1, 1)$ ?

What happens if  $P_n$  has only  $m < n$  zeros?

$$\xi_1, \dots, \xi_m \in (-1, 1)$$



Derivation of positivity:

We denote the Gauss points by  $\xi_j^n$   $j=1, \dots, n$  for an  $n$ -point G-L QF.

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

$\Rightarrow q_k \in P_{2n-2} \Rightarrow n$ -point G-L QF integrates  $q_k$  exactly!

$$0 < \int_{-1}^1 q_k(t) dt = \underbrace{\sum_{j=1}^n \omega_j^n \cdot q_k(\xi_j^n)}_{\text{QF}} = \omega_k^n \underbrace{q_k(\xi_k^n)}_{>0}$$

$\Rightarrow \omega_k^n > 0$ . This is true for all  $k=1, \dots, n$   $\square$ .

As for Chebychev polynomials, we again have a 3-term recursion formula:

Recursive formula for Legendre polynomials

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

$$P_{n+1}(t) := \frac{2n+1}{n+1} t P_n(t) - \frac{n}{n+1} P_{n-1}(t) \quad , \quad P_0 := 1, \quad P_1(t) := t. \quad (6.14)$$

Legendre polynomials:  
 $L^2$ -orth. polynomials

Chebychev polynomials:  
orth. polyn. w.r.t.  
weighted  $L^2$ .







Example: 2 functions 
 $\left\{ \begin{array}{l} \text{smooth} \\ \text{only cont.} \end{array} \right.$

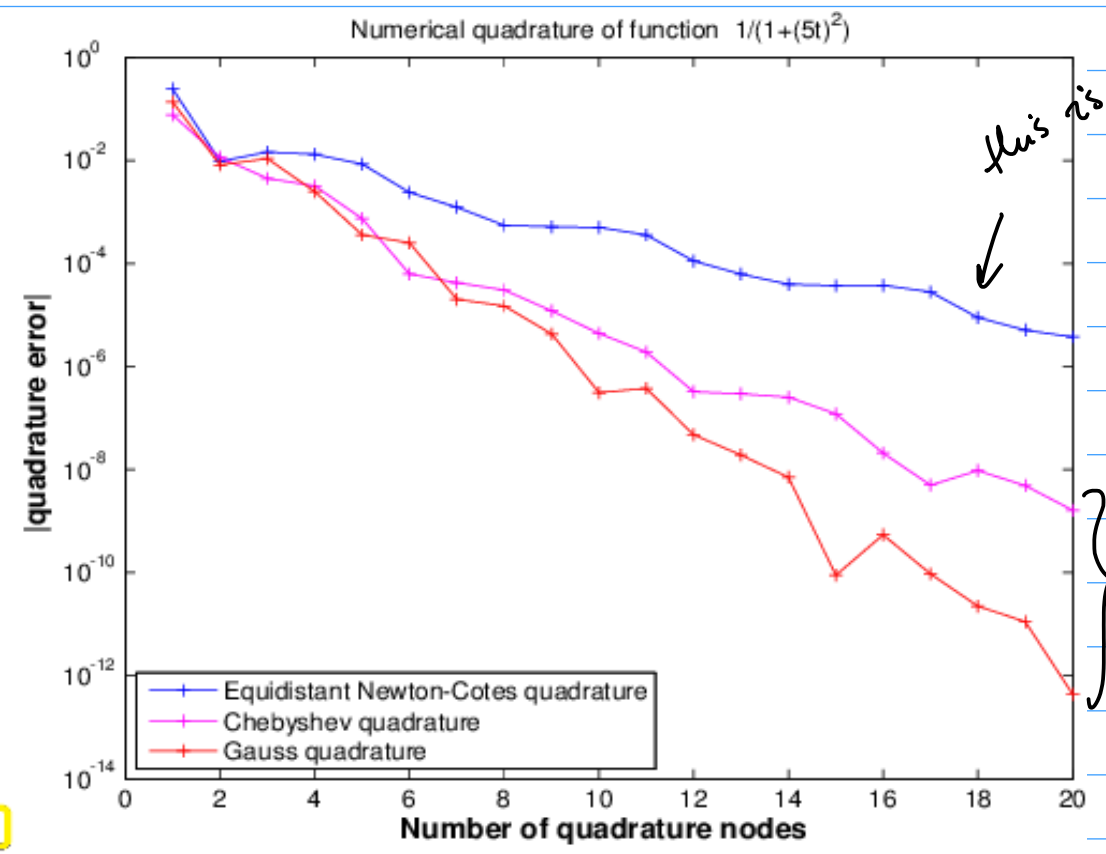


Fig. 268

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

this is not convergent  
 lin-log-plot  
 exponential conv.

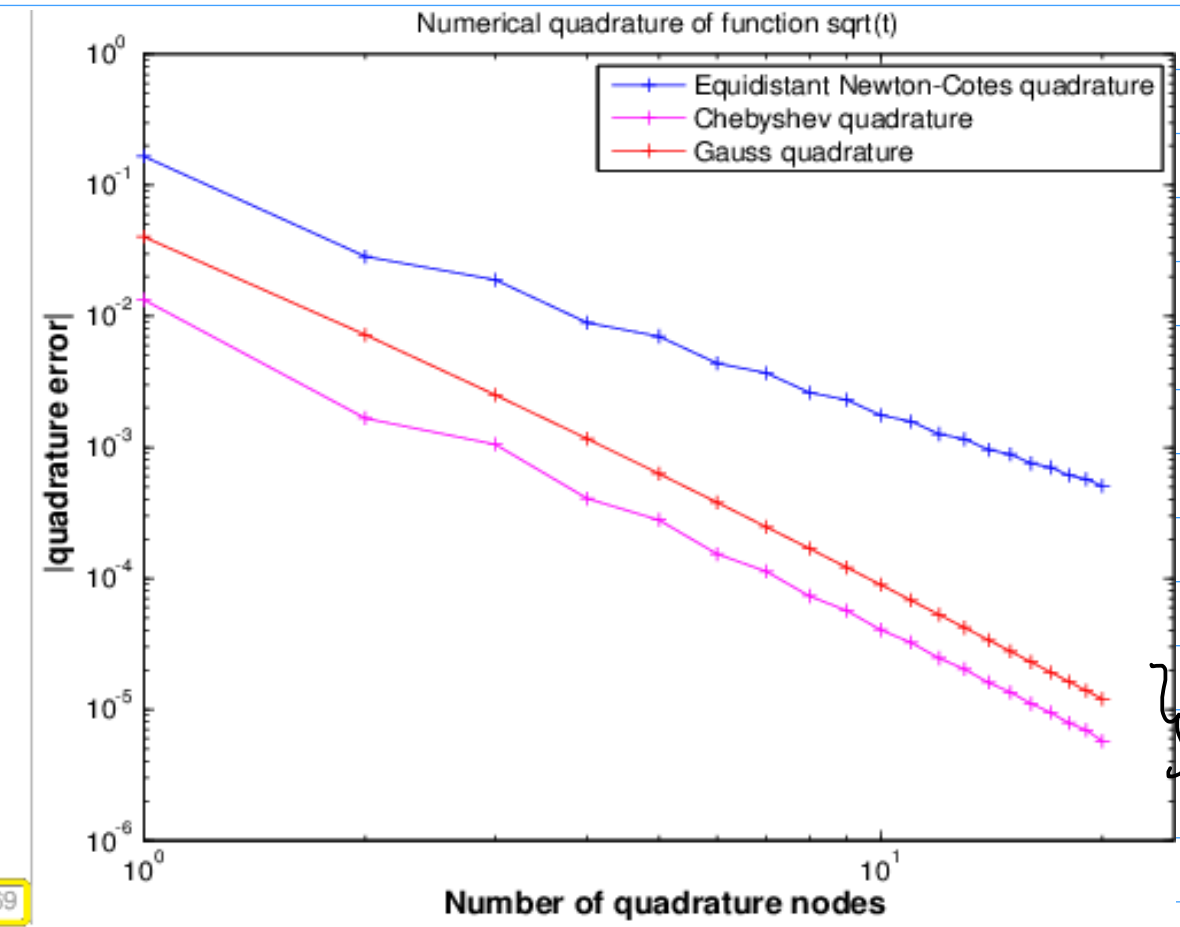


Fig. 269

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

log-log-plot  
 algebraic conv

Remark:

The integral of this particular function can be transformed:  
 substitute  $s = \sqrt{t}$



Suppose we had <sup>sharp</sup> exp. conv.:

$$E_n(f) = \mathcal{O}(\lambda^n) \Rightarrow E_n(f) \approx C \cdot \lambda^n$$

↑  
ind. of  $n$

$$\frac{C \cdot \lambda^{n_{\text{old}}}}{C \cdot \lambda^{n_{\text{new}}}} = g \Rightarrow$$

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

Here: only need to add a fixed number of nodes to improve the quadrature error by a factor  $g$ .

## Composite Quadrature

As for interpolation: introduce a mesh

& then apply a QF on each cell

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

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

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

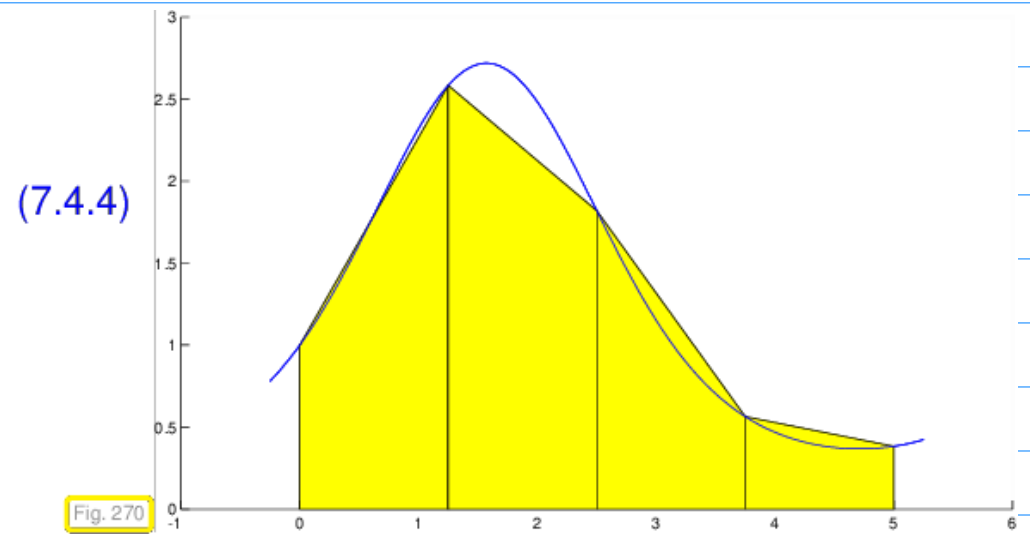
total number of function evaluations  $f$ :  $\sum_{j=1}^m n_j$

- Motivation:
- nodes are not freely choosable  
(then: equidistant + global polyn. interp. is a bad idea)
  - function is e.g. highly oscillatory

Examples:

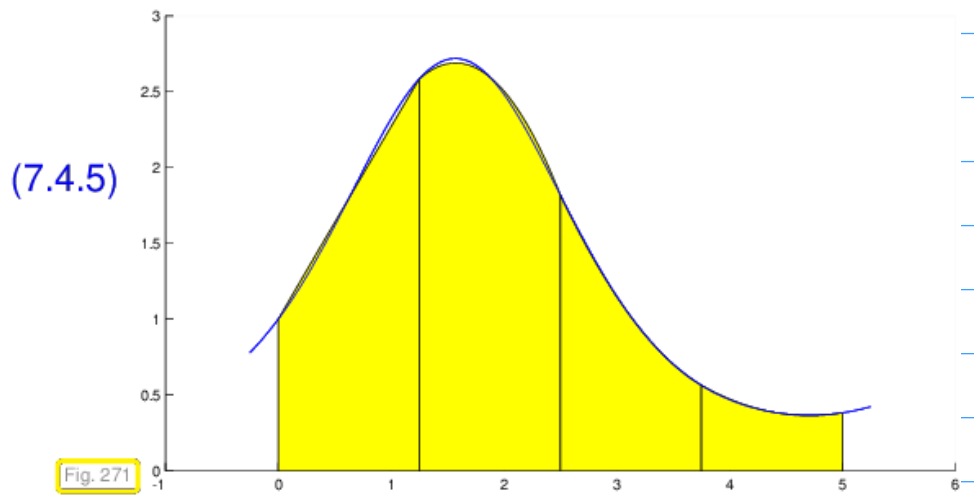
Composite trapezoidal rule, cf. (7.2.5)

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



Composite Simpson rule, cf. (7.2.6)

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



Error estimates for composite QF:

→ add errors on each  $I_j$

Suppose on each  $I_j$ : QF  $Q_n^j$  of order  $q$  & positive weights

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

$$\left| \int_{x_{j-1}}^{x_j} f(t) dt - Q_{n_j}^f(f|_{I_j}) \right| \leq C \cdot h_j^{\min\{r, q\}+1} \cdot \|f^{(\min\{r, q\})}\|_{L^\infty(I_j)} \quad (6.17)$$

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

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

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

$h_{\mathcal{M}} = \max_j h_j$

$\Rightarrow$  algebraic convergence in mesh width  $h_{\mathcal{M}}$

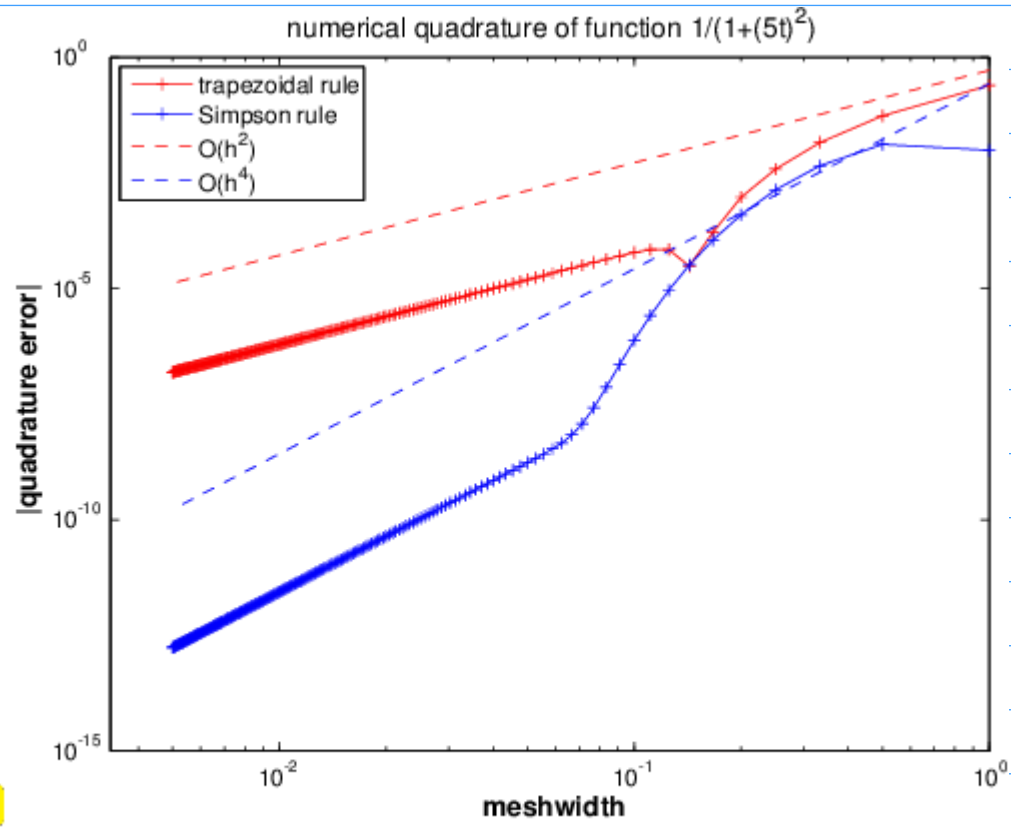
"h-convergence"

For  $r > q$ : algebraic convergence in  $h_{\mathcal{M}}$  of rate  $q$  (=order of the QF)

Example: Composite trapezoidal:  $q=2$

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

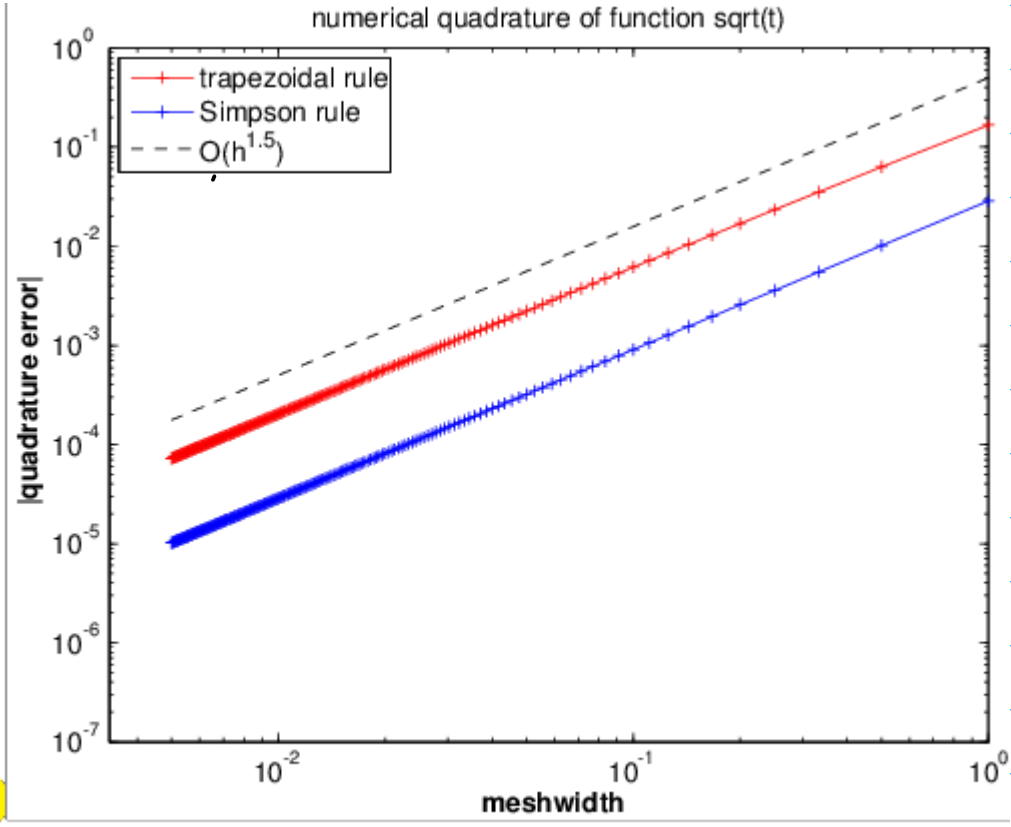
For suff. many times differentiable functions (i.e.  $r > q$ ):  $\underset{\text{trap.}}{\mathcal{O}(h^2)}$  vs.  $\underset{\text{Simpson}}{\mathcal{O}(h^4)}$



log - log - plot

Fig. 272

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



$O(h^{3/2})$

Fig. 273

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

Comparison of asymptotic rates of  
 / \  
 composite QF      global G-L QF

$f \in C^r([a, b])$ : Composite QF:  $\mathcal{O}(n^{-\min\{r, 9\}})$   
 Gauss QF:  $\mathcal{O}(n^{-r})$

$\Rightarrow$  Gauss is at least as good as composite QF  
 & achieves best possible rate

$f \in C^\infty([a, b])$ : Composite QF:  $\mathcal{O}(n^{-9})$  alg. conv.  
 Gauss QF:  $\mathcal{O}(1^n)$  exp. conv.  
 $\uparrow$   
 $\lambda \in (0, 1)$