→ Kenneth J. BEERS : "Numerical Methods for Chem. Eng." 2007
Cambridge Univ. Press

→ G. Beddard : "Applying Maths in the Chemical & Biomolecular Sci" 2009
Oxford Univ. Press

Permanent Idea : replace a difficult problem by a simpler one, being aware of consequences: error !

<u>Example</u> Total energy per mole of crystaline solid?

Debye theory:

Math. Modeling

$$E = \frac{9 N_0 k_B T}{x_m^3} \int_0^{x_m} \frac{x^3}{e^x - 1} dx \quad \text{with} \quad x = \frac{h\nu}{k_B T}$$

$$\nu_{max} = 8.06 * 10^{12} \frac{1}{s}$$

$$T = 1000\ K$$

$$E = \int_a^b f(x)\, dx$$

$$\int_a^b (x^5 - x^3)\, dx \ ; \quad \int_a^b \frac{x^3}{e^x - 1} dx$$

$$\underbrace{\int_a^b f(x)\, dx}_{\text{difficult}} \approx \underbrace{\sum_{k=1}^{n} f(c_k)\, w_k}_{\text{simple}}$$

Nodes of quadrature

weights of quadrature

difficult → simple

error?

Discretization

$|E_n - E|$ absolute error ; $\frac{|E_N - E|}{|E|}$ if $E \neq 0$, relative error

<u>Remark</u> Beware on the accumulation of round-off errors!

<u>Example</u> 1) $$J_n = \int_0^1 x^n e^{x-1} dx = x^n e^{x-1}\Big|_0^1 - n \int_0^1 x^{n-1} e^{x-1} dx =$$
$$= 1 - n J_{n-1}$$

$$J_n = 1 - n J_{n-1}$$

$$J_0 = \int_0^1 x^0 e^{x-1}\,dx = \int_0^1 e^{x-1}\,dx = 1 - \frac{1}{e}$$

Start $\Rightarrow$ $J_1 = 1 - 1 \cdot J_0 = \dots, \quad J_2 = \dots$

Exercise: write a loop (matlab) to print out $J_0, J_1, \dots, J_{30}$

compare $J_0, J_1, \dots, J_{30}$ to quad of matlab or your favourite quadrature rule

2) $x_{n+1} = 10 x_n - 9$

$x_0 = 1 \Rightarrow x_1 = 10 - 9 = 1 \Rightarrow x_2 = 10 - 9 = 1 \Rightarrow \dots \Rightarrow x_n = 1$

$\tilde{x}_0 = 1 + \varepsilon \Rightarrow x_1 = 10(1+\varepsilon) - 9 = 1 + 10 \cdot \varepsilon \Rightarrow$

$$x_n = 1 + 10^n \cdot \varepsilon$$

§1. Quadrature

$$\int_a^b f(t)\,dt = (b-a) \int_0^1 \overbrace{f((b-a)x + a)}^{g(x)}\,dx \Rightarrow \text{work only with } \int_0^1 g(x)\,dx$$

$$x = \frac{t-a}{b-a} \Rightarrow dx = \frac{dt}{b-a} \Rightarrow dt = (b-a)\,dx$$

$$J(g) = \int_0^1 g(x)\,dx \approx \sum_{k=1}^{n} g(c_k)\, w_k =: Q_n(g)$$

nodes $\in [0,1]$ weights $\in \mathbb{R}$

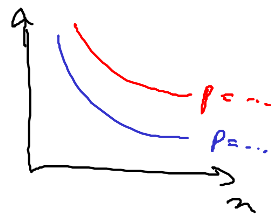
$$E(n) = | J(g) - Q_n(g) |$$

$E(n) \sim \dfrac{1}{n^p}$ with $p > 0$: algebraic convergence

$E(n) \sim q^n$ with $0 \le q < 1$: exponential convergence

Exercise plot $\dfrac{1}{n^p}$ for some values of p $\quad n = [0, 1, \dots, 10^2]$

q^n $\quad q$

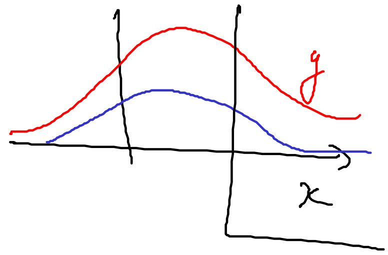


loglog

Def $\boxed{f(x) \in O(g(x)) \text{ for } x \to \infty}$ if there is a constant $M > 0$ s.t. $|f(x)| \le M\,|g(x)|$. LANDAU O-notation

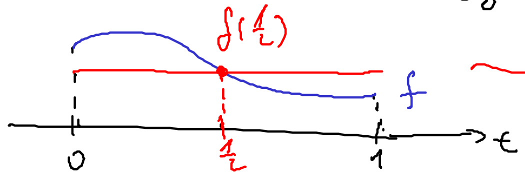
$E(n) \in O\left(\frac{1}{n^p}\right)$ alg. conv.

$E(n) \in O(q^n)$ exp. conv.



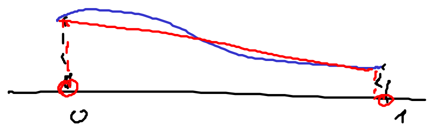
1) Nodes : aequidistant $\quad c_j = \frac{j}{n}$ for $j = 0, 1, 2, \dots, n$

Ex 1 node : midpoint rule: $\int_0^1 f(t)\,dt \approx f\left(\frac{1}{2}\right)$



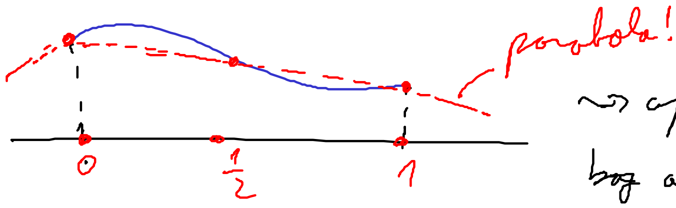
$\rightsquigarrow$ approximation of f with a constant

2 nodes : trapezoidal rule: $\int_0^1 f(t)\,dt \approx \frac{1}{2} f(0) + \frac{1}{2} f(1)$



$\rightsquigarrow$ approximation of f with a linear function

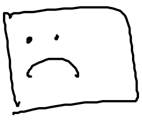
3 nodes: Simpson rule : $\int_0^1 f(t)\,dt \approx \frac{1}{6} f(0) + \frac{4}{6} f\left(\frac{1}{2}\right) + \frac{1}{6} f(1)$



$\rightsquigarrow$ approx. of f by a polynomial of degree 2!

$(n+1)$ nodes $\quad P_n(t) \approx f(t)$ Polynomial of degree n

$\rightarrow$ integrate exactly $\int_0^1 P_n(t)\,dt$



for large n!

2) Gaussian-Quadrature : choose n weights and n nodes s.t.

$E(n) = 0$ for f = Polynomial of degree $2n-1$

$\rightarrow$ $2n$ coefficients

$$\int_{-1}^{1} f(x)\,dx \approx f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

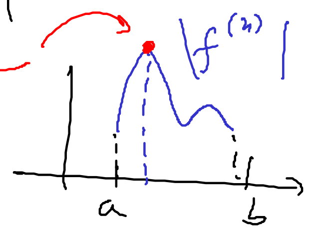
3) Clenshaw-Curtis

Note: Smoothness (= differentiability) of f is essential!

Quadrature formula which is exact for polynomials of degree n and f which is n times cont. differentiable:

$\left[\int_a^b f(x)\,dx\right]$ $\qquad f', f'', \dots, f^{(n)}$ continuous

$$E(f) \le C \cdot \frac{1}{n!} \underline{(b-a)}^{n+1} \max_{x\in[a,b]} |f^{(n)}(x)|$$

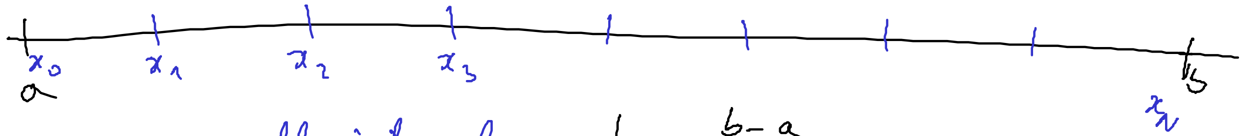


$$n! = 1 \cdot 2 \cdot 3 \cdot 4 \cdots n$$

Note: if $b-a$ = length of the integration interval is large

$\Rightarrow$ large error

$\downarrow$ Idea! Divide and conquer!



$\Rightarrow$ N small intervals $\qquad h = \frac{b-a}{N} < 1$

Then apply the quadrature rule on each of the intervals $[x_k, x_{k+1})$ for $k = 0, 1, \dots, N-1$

$$\Rightarrow \int_a^b f(t)\,dt = \sum_{k=0}^{N-1} \int_{x_k}^{x_{k+1}} f(t)\,dt \approx \sum_{k=0}^{N-1} Q_n(f, x_k, x_{k+1})$$

composite quadrature rule

(Zusammengesetzte Quadratur-Regel)

Ex Trap:
$$\int_a^b f(t)\,dt = \frac{h}{2}f(a) + \boxed{\frac{h}{2}f(x_1) + \frac{h}{2}f(x_1)} + \boxed{\frac{h}{2}f(x_2) + \dots} + \boxed{\frac{h}{2}f(x_{N-1})} + \frac{h}{2}f(b)$$

$$= \frac{h}{2}\left(f(a)+f(b)\right) + h\sum_{k=1}^{N-1} f(x_k)$$

Th. $h = \max_{k=0,1,\dots,N} |x_{k+1}-x_k|$, Quadrature rule exact for polynomials of degree $p-1$ (n)

Then there is $C>0$ s.t.

order of convergence

$$\left| \int_a^b f(t)\,dt - Q(f) \right| \le C\cdot h^{p\,(n)} \max_{t\in[a,b]} \left| f^{(p)\,(n)}(t) \right|$$

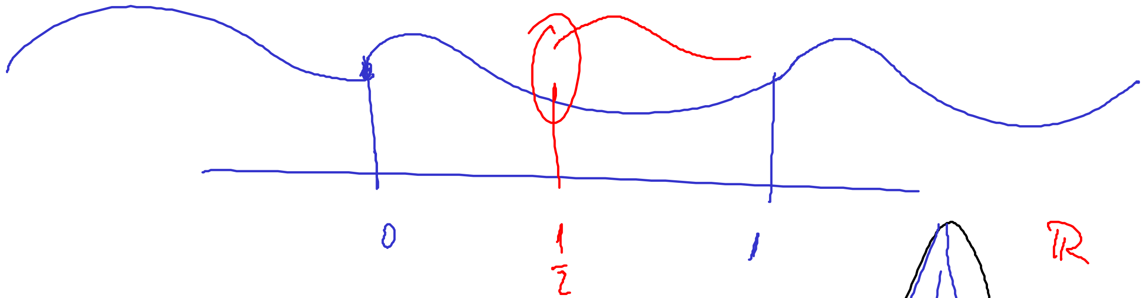
error $O(h^p)$

<u>Exercise</u> Plot error for

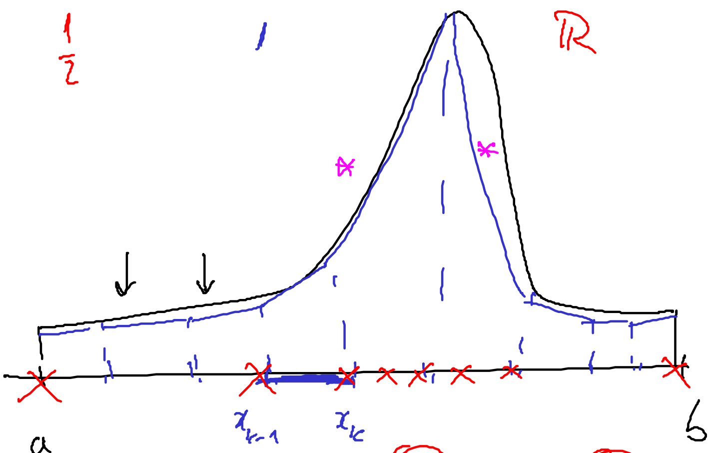
1) $f_1(t) = \dfrac{1}{1+(5t)^2}$ on $[0,1]$

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

3) $f(t) = \dfrac{1}{\sqrt{1-a\sin(2\pi t-1)}}$ with $0<a<1$ on $[0,1]$ on $[0,\frac{1}{2}]$



<u>Adaptivity</u>



error on $[x_{k-1}, x_k]$ is $\frac{1}{6}(x_k - x_{k-1})^3 \max_{x\in[x_{k-1},x_k]} |f^{(2)}(x)|$ [trap. rule]

$*$: f varies a lot $\Rightarrow$ $f^{(2)}$ is large there!

more efficient: put points/intervalls only there where the function varies a lot

Even better: locally refine the grid (more intervals) there where the error is large

How to estimate the local error

Q_1, Q_2 of different orders

$$|I - \underline{Q_1(f)}| \approx c h^2$$

$$|I - \underline{Q_2(f)}| = c h^4$$ much more exact $\Rightarrow$ use $Q_2(f)$ as an accurate estimate of I:

local error $= |I - Q_1(f)| \simeq \underline{|Q_2(f) - Q_1(f)|}$ = estimator of local error