Numerical simulation

Numerical simulation is the third pillar of science and technology besides theory and experiment to understand the world around us, e.g., if

- properties/structures are not experimentally accessible
- experiments are expensive/time-consuming (and thus only few can be done)
- theories have to checked by testing their predictions

- engineering: structural and fluid mechanics, optimization, material science, propagation of electromagnetic waves, . . .
- physics: astrophysics, quantum mechanics
- chemisty: drug development, structural analysis of proteines, . . .
- medicine: computer tomography, i.e., inverse problems
- geology: seismic analysis/inverse problems
- ecology: climate calculations, weather predictions, . . .

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Numerics and the big picture

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the bigger picture:

reality → math. model → numer. simulation → assessment

some core questions in numerics:

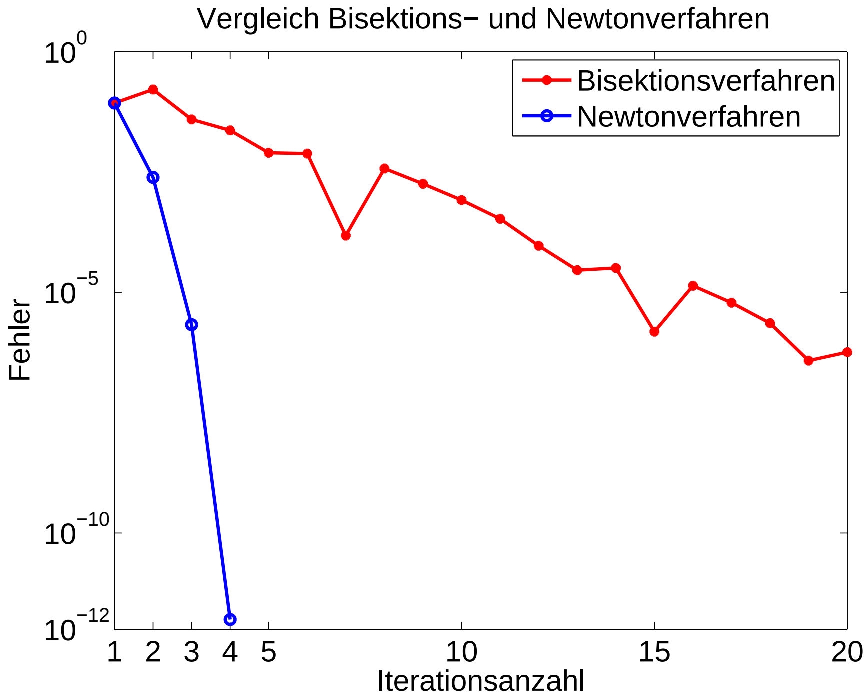
- convergence of algorithms; *a priori* error estimates
- efficiency of algorithms
- reliability of algorithms; *a posteriori* error estimation

convergence and efficiency: zeros of a function

example: bisection method and Newton's method for solving $x^2 - 2 = 0$

$$x_{i+1} := \frac{1}{2}\left(x_i + \frac{2}{x_i}\right), \qquad i = 0, 1, \ldots,$$

	Newton's method ($x_0 = 2$)	bisection method ($I_0 = [1, 2]$)
x_1	1.5	1.5
x_2	**1.41**6666666666667	**1**.250000000000000
x_3	**1.41421**5686274510	**1**.375000000000000
x_4	**1.41421356237**4690	**1.4**37500000000000
$\vdots$		$\vdots$
x_{10}		**1.41**5039062500000
$\vdots$		$\vdots$
x_{15}		**1.41421**5087890625
$\vdots$		$\vdots$
x_{37}		**1.41421356237**697
	quadr. convergence	linear convergence



cos per step:

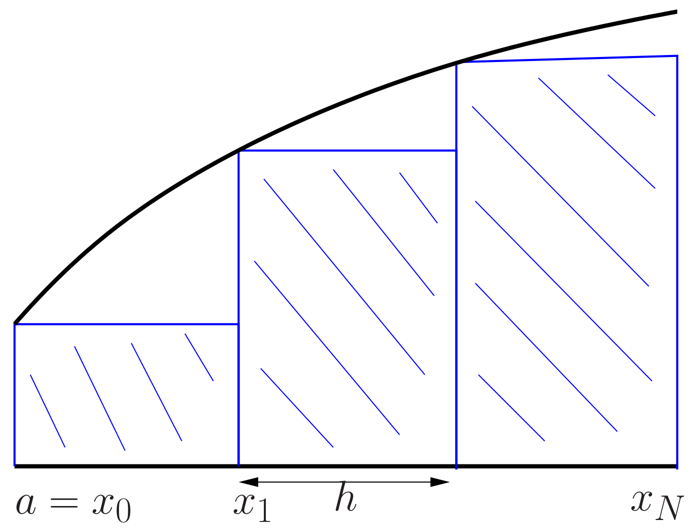
bisection method	1 addition, 1 division by 2, 1 multiplication, 1 comparison
Newton's method	1 addition, 1 division by 2, 1 division

convergence, efficiency, error estimation for quadrature

goal: approximate $\int_a^b f(x)\,dx$, where $f \in C^2([a,b])$.
partition $[a,b]$ in N subinterals $[x_i, x_{i+1}]$ of length h with

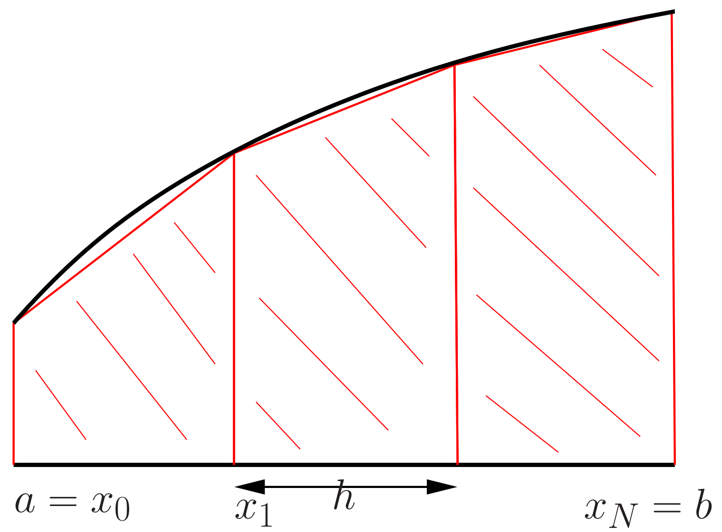
$$x_i = a + ih, \qquad i = 0, \ldots, N, \qquad h = \frac{b-a}{N}$$

box rule



$$R(h) := \sum_{i=0}^{N-1} h f(x_i)$$

trapezoidal rule



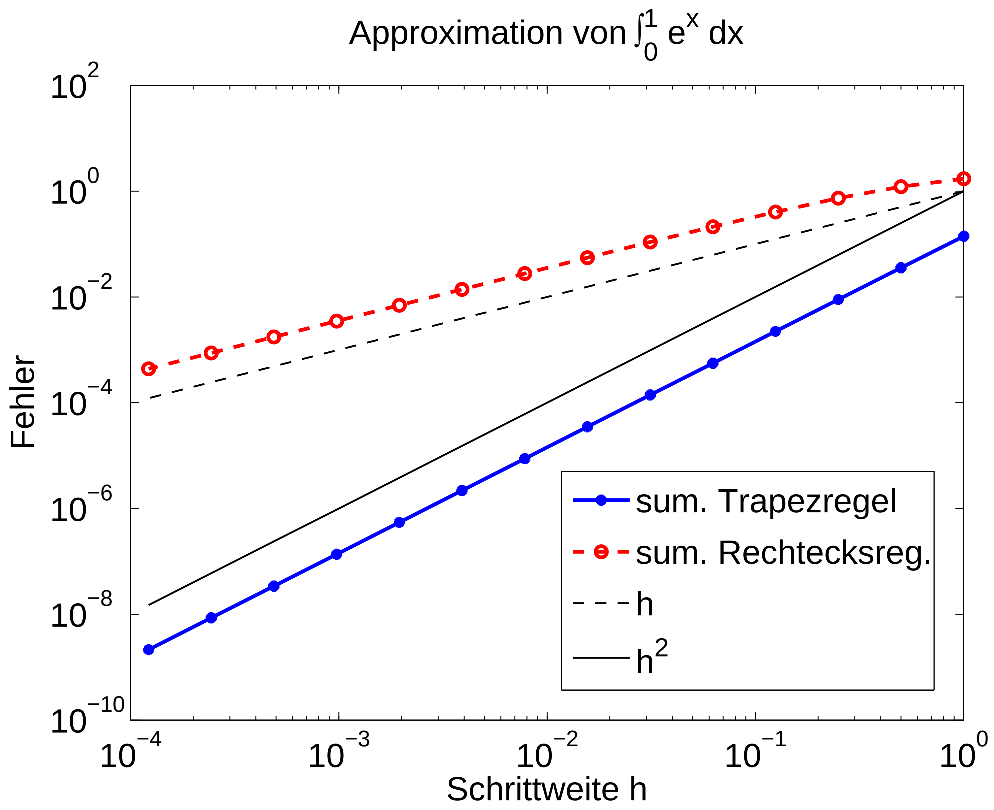
$$T(h) := \sum_{i=0}^{N-1} \frac{h}{2} \left[f(x_i) + f(x_{i+1}) \right]$$

convergence of the trapezoidal and box rules

a priori estimates:

$$\left| \int_a^b f(x)\,dx - R(h) \right| \leq \frac{b-a}{2} h \|f'\|_{C([a,b])}$$

$$\left| \int_a^b f(x)\,dx - T(h) \right| \leq \frac{b-a}{6} h^2 \|f''\|_{C([a,b])}$$



efficiency of the trapezoidal rule (as opposed to the box rule)

number of function evaluations F is:

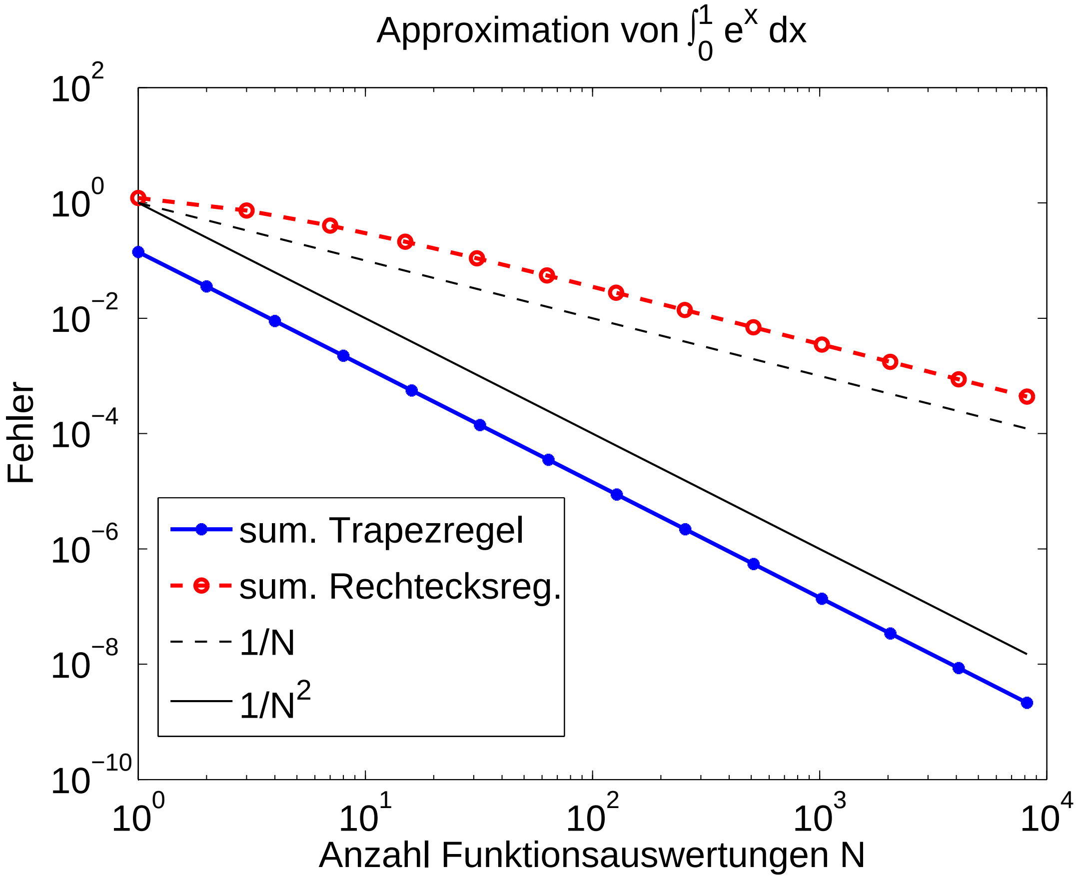
$$
\begin{aligned}
F &= N-1 \text{ for box rule} \\
F &= N \text{ for trapezoidal rule}
\end{aligned}
$$

In both cases $F \approx N$. From $h = \frac{b-a}{N}$ we get:

$$
\begin{aligned}
\left| \int_a^b f(x)\,dx - R(h) \right| &\leq C_{box} F^{-1} \|f'\|_{C([a,b])} \\
\left| \int_a^b f(x)\,dx - T(h) \right| &\leq C_{trap} F^{-2} \|f''\|_{C([a,b])}
\end{aligned}
$$

efficiency of the trapezoidal rule (as opposed to the box rule)

conclusion: the trapezoidal rule is more efficient than the box rule in the sense that (at least asymptotically) fewer function evaluations are required to achieve a given accuracy.



error estimation for box rule using extrapolation

fact: $\int_a^b f(x)\,dx - R(h) \approx Ch$ for all sufficiently small h and suitable C.

idea: compute C. To that end, assume $\int_a^b f(x)\,dx - R(h) = Ch$. Then:

$$\begin{aligned}\int_a^b f(x)\,dx - R(h) &= Ch \\ \int_a^b f(x)\,dx - R(h/2) &= Ch/2\end{aligned}$$

Hence, by subraction: $R(h/2) - R(h) = Ch/2$. Therefore, we obtain

$$\underbrace{\int_a^b f(x)\,dx - R(h)}_{\text{not computable}} \approx Ch = \underbrace{2\,[R(h/2) - R(h)]}_{\text{computable!}}$$

error estimation for box rule using extrapolation

We have obtained:

$$\underbrace{\int_a^b f(x)\,dx - R(h)}_{\text{true error: not computable}} \approx Ch = \underbrace{2\,[R(h/2) - R(h)]}_{\text{error estimator: computable!}}$$

numerical example:

h	2^0	2^{-1}	2^{-2}	2^{-3}	2^{-4}	2^{-5}	2^{-6}	2^{-7}	2^{-8}	2^{-9}
$2\frac{R(h/2)-R(h)}{\int_0^1 e^x\,dx - R(h)}$	0.90	0.95	0.98	0.99	0.995	0.997	0.99	0.999	0.9997	0.9998

reliability, error estimation

Sleipner oil platform 1991

damage: \$ 700,000,000

reason: underestimation of the forces inside a part during the numerical simulation

simulation: commercial FE-code NASTRAN without error estimation and adaptive control of the simulation to ensure reliability of the results