4.10.2022

Introduction to Numerics/Numerical Computation

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TU Wien
Institute for Analysis and Scientific Computing

Formalities

Format

VU: lecture with integrated exercise

- Visual Computing 2h (blocked until christmas as 2h lecture + 1h exercise)
- Informatics/Geodesics 3h (2h lecture + 1h exercise)
- CSE 4h (3h lecture + 1h exercise)

TUWEL course! - you can self-enroll

In person format

- Attendance in the lecture hall at all times possible
- No camera in the lecture hall – unfortunately, no streaming

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Dates

1h academic = 45 minutes

Dates - Lecture

- Tuesday 8:15-9:55 (2h academic, including 10min break) for everybody!
  - room: FH HS 3
- Wednesday 9:15-10:00 (1h academic) CSE only!
  - room: FH HS 4 (only tomorrow 5.10.)
  - room: Sem.R. DA grün 03 B (Freihaus, 3rd floor green)

Dates - Exercise

various groups (register in TISS!!), either

- Monday 10:00-11:00
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note: we do a full hour of exercise, to account for missing weeks!

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Exercises start on 17.10./18.10.!

Checkmark format

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- Checkmarks done in TUWEL
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Tests

Tests

Two written tests

- Friday 25.11.2022 room and time TBA
- Thursday 26.01.2023

Re-test

- only for those who miss one test or did fail not to horribly!
- Friday 24.02.2023

Grading

- Total 100 points
  - Exercise part: max. 34 points
  - Each test: max. 33 points

Grading (positive)

- more than 60% of checkmarks
- overall positive grade for your presentation
- overall > 50 points
- at least > 33 points in the written examinations

Final grades: $(50, 62.5]$ grade 4, $(62.5, 75]$ grade 3, $(75, 87.5]$ grade 2, $(87.5, 100]$ grade 1

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Course Materials

- Everything uploaded to TUWEL
- Exercise sheets one week before exercise online
- Lecture notes from Prof. Melenk from last year used

Why take this lecture?

Numerical simulation

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, material science, wave propagation, ...
- physics: astrophysics, quantum mechanics
- chemisty, medicine: drug development, structural analysis of proteines, CT, ...
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Numerics

Numerics

Numerics is concerned with the development and analysis of algorithms that realize mathematical calculations and methods on computers.

the bigger picture:

reality $\longrightarrow$ math. model $\longrightarrow$ numer. simulation $\longrightarrow$ assessment

some core questions in numerics:

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

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Convergence and efficiency: zeros of a function

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

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

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

Convergence and efficiency: zeros of a function

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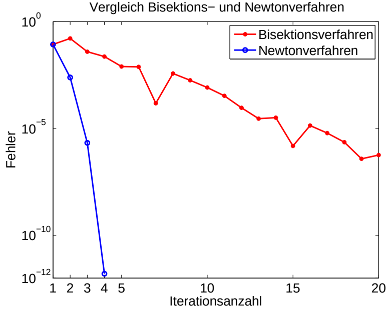
	Newton's method ($x_0 = 2$)	bisection method ($I_0 = [1, 2]$)
x_1	1.5	1.5
x_2	**1.41**6666666666667	**1**.250000000000000
x_3	**1.414215**686274510	**1**.375000000000000
x_4	**1.41421356237**4690	**1.4**37500000000000
$\vdots$		$\vdots$
x_{15}		**1.414215**087890625
x_{37}		**1.41421356237**697
	quadr. convergence	linear convergence



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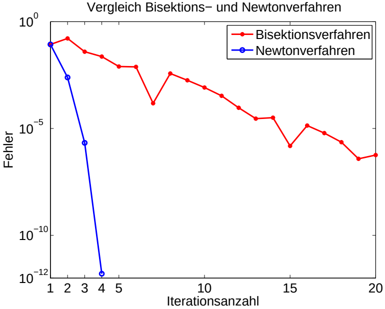

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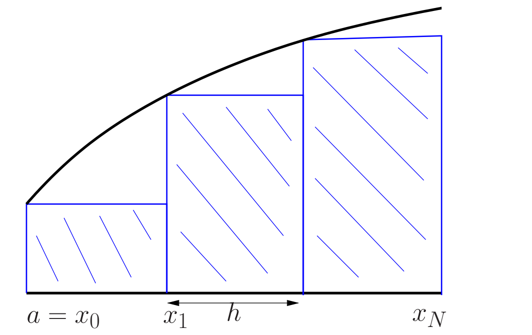
Numerical integration: convergence, efficiency, error estimation

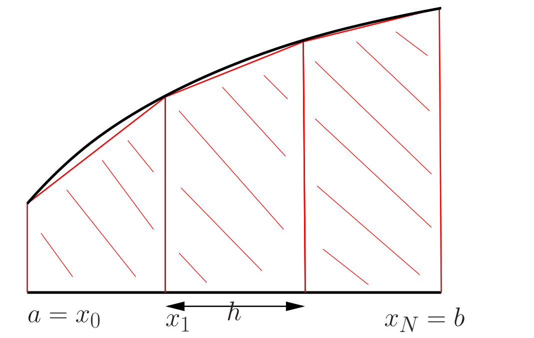
goal: approximate $\int_a^b f(x)\,dx$ partition $[a,b]$ in N intervals $[x_i, x_{i+1}]$ of length h

box rule



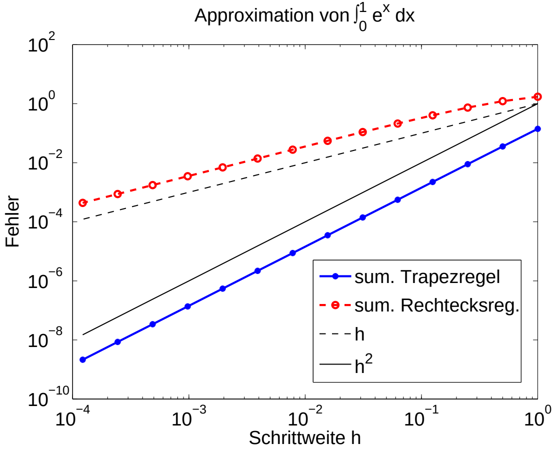
$$R(h) := \sum_{i=0}^{N-1} h f(x_i)$$

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:

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

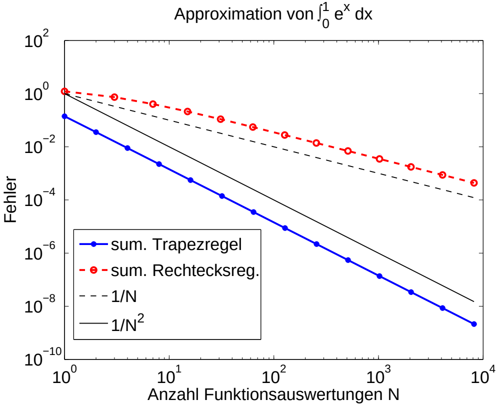
$$\left|\int_a^b f(x)\,dx - T(h)\right| \leq \frac{b-a}{6} h^2 \|f''\|_\infty$$

Efficiency of the trapezoidal rule

number of function evaluations F is

- $F = N - 1$ for box rule
- $F = N$ for trapezoidal rule

In both cases $F \approx N \sim h^{-1}$



Thus, trapezoidal rule is more efficient (less evaluations for same accuracy)!

Error estimation for box rule (a-posteriori)

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

idea: compute C. We assume equality above, 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

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

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Bad numerics

Sleipner oil platform 1991

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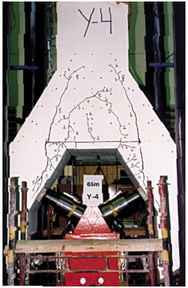
damage: \$ 700,000,000

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

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



Contents of the lecture

Content I

- Polynomial interpolation of function f

$$\text{find polynomial } p \text{ s. t. } p(x_i) = f(x_i)$$

  e.g. used for plotting!

- Numerical integration

$$\text{approximate } \int_a^b f(x)dx$$

- Newton's method for zeros of non-linear equations

Content II

- Solution of linear systems of equations $Ax = b$
  - Gaussian elimination
  - least-squares methods (optimization) for over-/underdetermined systems
  - iterative methods for efficient approximative solution
- Computation of eigenvalues of matrices, i.e., find

$$\lambda, v \text{ s.t. } Av = \lambda v$$

- Numerical solution of differential equations