Technische Universität Graz
Institut für Theoretische Physik

Name: [redacted]

COMPUTERMETHODEN DER TECHNISCHEN PHYSIK
Exam 1 WS 2023/2024

01.02.2024

This written exam for the lecture *Computational Methods in Technical Physics* consists of three exercises based on the numerical methods explained during the semester. You are supposed to show your calculation for every derivation and calculation in the exam, but not for the multiple choice questions.

You have two hours to complete the solutions.

The use of books and notes on paper is allowed. The use of electronic devices is not allowed.

Good luck!

1 Short questions (25 points)

For the multiple choice questions, there is only one correct answer, unless noted otherwise.

[redacted]

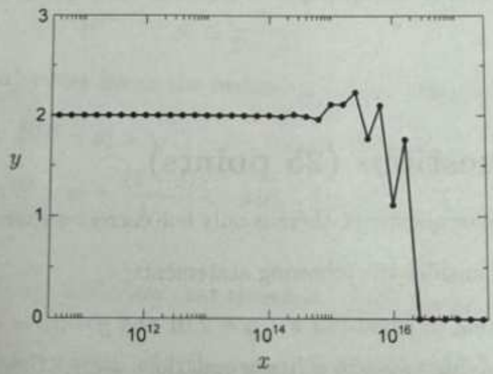
(ii) [redacted]

f. Which of the following statements is true?

Multiple Choice
aus rechtlichen Gründen geschwärzt

(iii) **(5 points)** The following figure shows the result of a numerical calculation of

$$y = x \ln\left(1 + \frac{1}{x}\right) - x \ln\left(1 - \frac{1}{x}\right).$$



Explain the observed behavior.

(iv) **(5 points)** Explain why the signal length for fast Fourier transform needs to be equal to 2^N with N being an integer number.

[redacted]

(v) **(5 points)** The two absolute smallest eigenvalues of the matrix

$$A = \begin{bmatrix} 3 & 2 & 4 \\ 2 & 0 & 2 \\ 4 & 2 & 3 \end{bmatrix}$$

have equal magnitude. For each of the following algorithms, *discuss* whether they can be used to determine all eigenvectors and eigenvalues of A.

[redacted] Jacobi rotations [redacted]

The power method (von Mises iteration) [redacted]

The QR algorithm [redacted]

Application of Gershgorin's theorem [redacted]

2 Euler integration (25 points)

Consider the initial value problem

$$\dot{x}(t) = \lambda x(t) \quad \text{and} \quad x(t_0) = x_0 = 2, \tag{1}$$

with $\lambda \in \mathbb{R}$.

(i) **(5 points)** Write down the Taylor expansion of $x(t)$ in the position $t_{n+1} = t_n + h$ up to second order.

(ii) **(5 points)** Apply Euler's method (first-order Taylor approximation) to derive $x_n = x(t_n)$ in terms of x_0, n, λ, and the stepsize h.

(iii) **(5 points)** For $\lambda < 0$ the solution converges to $x(t) = 0$ for $t \to \infty$. What condition on h ensures that $|x_n| \to 0$ as $n \to \infty$? Compare the cases $\lambda = -1$ and $\lambda = -100$.

(iv) **(5 points)** Write down a second-order Taylor approximation for x_n in terms of x_0, n, λ and the stepsize h.

(v) **(5 points)** What is the condition on h that ensures $|x_n| \to 0$ as $n \to \infty$ when using the second-order Taylor approximation?

3 Error bound of the fixed-point iteration (30 points)

Consider the iterative process

$$x^{(p+1)} = f(x^{(p)}) + \varepsilon^{(p)}. \tag{2}$$

The function $f(x) : \mathbb{R} \to \mathbb{R}$ satisfies

$$|f(x) - a| \leq \beta |x - a| \quad \text{for all } x \in \mathbb{R}, \tag{3}$$

where $a \in \mathbb{R}$ is a constant and $0 < \beta < 1$. Furthermore, the truncation error

$$|\varepsilon^{(p)}| \leq \gamma \quad \text{for all } p, \tag{4}$$

with γ being a real-valued positive constant.

(i) **(5 points)** Show that $f(a) = a$. Derive an inequality for $|x^{(p+1)} - a|$ in terms of $x^{(p)}$, β and γ and explain what may happen when $(1-\beta)|x^{(p)} - a| < \gamma$.

We split the domain of x in two regions, one near a and one far away from a.

(ii) **(5 points)** Inside the region $|x^{(p)} - a| \leq \gamma/(1-\beta)$, show that

$$|x^{(p+1)} - a| \leq \frac{\gamma}{1-\beta},$$

so the sequence $\{x^{(p)} - a\}$ never leaves the region once it has entered.

(iii) **(5 points)** In the region $|x^{(p)} - a| > \gamma/(1-\beta)$, we can write

$$|x^{(p)} - a| = \frac{(1+\delta)\gamma}{1-\beta} \quad \text{with} \quad \delta > 0.$$

Show that

$$|x^{(p)} - a| - \gamma > \beta |x^{(p)} - a| \quad \text{and show that therefore} \quad |x^{(p+1)} - a| < |x^{(p)} - a|.$$

(iv) **(5 points)** Use part (iii) to explain why the sequence $\{|x^{(p)} - a|\}$ converges to a limit b if $|x^{(p)} - a| > \gamma/(1-\beta)$ for all finite p.

(v) **(5 points)** Suppose the limit is given by $b = \gamma/(1-\beta) + \delta$ with $\delta > 0$. Since $\beta < 1$, for some q we must have

$$|x^{(q)} - a| < \frac{\gamma}{1-\beta} + \frac{\delta}{\beta}.$$

Show that that means $|x^{(q+1)} - a| < b$. Derive the value of b in terms of γ and β from the contradiction.

(vi) **(5 points)** Explain the practical relevance of the results of parts (ii) and (v) for the sequence $\{x^{(p)}\}$ generated by Eq. (2) in terms of a, γ, β, and $\varepsilon^{(p)}$.