Technische Universität Graz
Institut für Theoretische Physik

# COMPUTERMETHODEN DER TECHNISCHEN PHYSIK
## Exam 2 WS 2019/2020
## *Lockdown Edition*

**13.05.2020**

This written exam for the lecture *Computational Methods in Technical Physics* consists of four exercises based on the numerical methods explained during the semester. Answers to the exercises can be submitted in the form of a text file or email text. As an example, the answer to a multiple choice question can be given as

```
1(i):  a
```

Whenever values are asked, you do not need to explain the calculation in your answer. There is no need to format any compex mathematics. Simple mathematical expressions, such as the value of $\pi$, $\frac{1}{2}$, or $|A|$ can be written as `pi`, `1/2` and `|A|`.

You have three hours to complete the solutions. The time starts at the moment you received the email containing this exam. To submit your solutions, reply to the email within three hours of receiving it.

The use of books, lecture notes and internet is allowed, but communication and collaboration with third parties are not. In case of suspicion, an additional oral exam can be requested.

During the exam, questions about the exam can be sent by email to bonthuis@tugraz.at.

Good luck!

# 1 Short questions

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

(i) **(4 points)** A $n$-point running average of a data set can be described as a convolution with the block function

$$f(x_i) = \begin{cases} 0 & \text{if } i < 0 \\ 0 & \text{if } i \geq n \\ 1/n & \text{else.} \end{cases}$$

Explain in words how a running average can be calculated using Fourier transforms.

(ii) **(4 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. Which of the following techniques can be used to determine the eigenvectors and eigenvalues of $A$? (multiple answers possible)

(a) QR decomposition

(b) Jacobi rotations

(c) Power method (von Mises iteration) together with deflation

(d) None of the above

(iii) **(4 points)** Given a data set $y_i(x_i)$ for $i = 1 \ldots n$. Solving the equations

$$y_i = \sum_{j=1}^{n} c_j x_i^{j-1}$$

for the coefficients $c_j$ corresponds to

(a) a polynomial interpolation

(b) a polynomial fit

(c) a quadratic spline interpolation

(d) a nonlinear least-squares fit

(iv) **(4 points)** Explain how high-frequency noise can be suppressed using interpolation of a data set.

(v) **(4 points)** Explain the difference between an explicit and an implicit numerical integration method, including the differences in the numerical implementation.

(vi) **(4 points)** A rational number is written in the decimal system using 5 digits, *i.e.* in the format $0.d_1d_2d_3d_4d_5 \cdot 10^n$ with $d_1 \neq 0$. The number is truncated after the fifth digit. The maximum *relative* rounding error is equal to

(a) $1 \cdot 10^{-5}$

(b) $5 \cdot 10^{-5}$

(c) $1 \cdot 10^{-4}$

(d) $5 \cdot 10^{-4}$

## 2 Solving a system of linear equations

Consider the system of linear equations

$$\begin{aligned} v + 2w &= 4 \\ 2v - w &= 3. \end{aligned} \tag{1}$$

Using $\boldsymbol{x} = (v, w)$, Equation (1) can be rewritten as $LU\boldsymbol{x} = \boldsymbol{y}$, with $L$ being a lower-diagonal matrix with ones on the diagonal, and $U$ being upper-diagonal.

(i) **(5 points)** What is the value of $U_{22}$ (the lower right element of the matrix $U$)?

(ii) **(5 points)** Explain in words how the $LU$ decomposition can be used to solve Equation (1).

Alternatively, an iterative algorithm can be used. The iterative scheme can be written as

$$\boldsymbol{x}_{p+1} = B\boldsymbol{x}_p + \boldsymbol{c}. \tag{2}$$

(iii) **(5 points)** What is the condition for $B$ to guarantee that the iteration converges?*

(iv) **(5 points)** Which of the following iterative algorithms is guaranteed to converge to the correct solution?

(a)
$$\begin{aligned} v_{p+1} &= 4 - 2w_p \\ w_{p+1} &= -(3 - 2v_p) \end{aligned}$$

(b)
$$\begin{aligned} v_{p+1} &= (3 + w_p)/2 \\ w_{p+1} &= (4 - v_p)/2 \end{aligned}$$

(c)
$$\begin{aligned} v_{p+1} &= 4 - v_p - 2w_p \\ w_{p+1} &= -(3 - 2v_p + w_p) \end{aligned}$$

(d)
$$\begin{aligned} v_{p+1} &= 4 + 2w_p \\ w_{p+1} &= -3 + 2v_p \end{aligned}$$

(v) **(5 points)** Explain in words why your answer to question (iv) is guaranteed to converge to the right values.

*Hint: Inserting the solution $\boldsymbol{x}_{exact}$ into Equation (2) leads to a relation between $\boldsymbol{x}_{p+1} - \boldsymbol{x}_{exact}$ and $\boldsymbol{x}_p - \boldsymbol{x}_{exact}$.

## 3 Numerical integration

Consider the integral

$$F = \int_0^{\pi} \sin x \, dx. \tag{3}$$

(i) **(2 points)** What is the exact value of $F$?

The integral can be approximated using the equation $F = \displaystyle\int_a^b f(x)dx = F_n + \xi_n$, with $\xi_n$ being the numerical error, and

$$\begin{aligned} F_n &= \frac{h}{3}\left(f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \ldots + 4f(x_{n-1}) + f(x_n)\right), \\ h &= (b-a)/n, \\ x_i &= a + ih. \end{aligned} \tag{4}$$

(ii) **(4 points)** Calculate $F_n$ for the integral of Equation (3) for $n = 2$.

(iii) **(5 points)** What is the order of the error $\xi_n$ in terms of the number of steps $n$?

- (a) $\mathcal{O}(n^{-2})$
- (b) $\mathcal{O}(n^{-3})$
- (c) $\mathcal{O}(n^{-4})$
- (d) $\mathcal{O}(n^{-5})$

By $g(x)$ we denote the second order polynomial (quadratic) interpolation to the function $f(x) = \sin x$ in the interval $0 \le x \le \pi$.

(iv) **(5 points)** Which of the following functions corresponds to $g(x)$?

- (a) $4x(\pi - x)/\pi^2$
- (b) $-0.42x^2 + 1.3x - 0.05$
- (c) $1 - |\frac{2x}{\pi} - 1|$
- (d) $-\frac{4x^2}{\pi^2} + \frac{4x}{\pi} + 1$

(v) **(5 points)** Analytically calculate the exact value of the integral $G = \displaystyle\int_0^{\pi} g(x)dx$.

(vi) **(5 points)** Is there a relation between $F_2$ from question (ii) and $G$ from question (v)? Explain your answer in words based on the background of the approximation used in Equation (4).

# 4 The square root of three

Consider a numerical algorithm for calculating $x_{exact} = \sqrt{3}$.

(i) **(6 points)** The Newton-Raphson algorithm is based on iteratively solving the equation $x^2 - 3 = 0$ using

$$x_{p+1} = \frac{x_p^2 + 3}{2x_p},$$

where $p$ is the iteration number. Explain in words how the Newton-Raphson method works in theory, as well as the steps that need to be taken in practice to solve the equation numerically.

(ii) **(6 points)** Define the value $A$ as

$$A = \frac{|x_{p+1} - x_{exact}|}{|x_p - x_{exact}|^2}.$$

Which of the following statements is true when $x_p$ approaches $x_{exact}$?

(a) $A$ decreases quadratically

(b) $A$ converges to a constant value

(c) $A$ diverges to infinity

(d) $A$ approaches zero

(iii) **(6 points)** Explain in words what your answer to question (ii) signifies for the convergence of the Newton-Raphson method.

(iv) **(7 points)** An alternative to the Newton-Raphson method is to use the secant (*regula falsi*) method. Which of the following iterative equations can be used to find the square root of three?

(a) $x_{p+1} = \frac{x_p x_{p-1} + 3}{x_p + x_{p-1}}$

(b) $x_{p+1} = \frac{2x_p^2 + x_p x_{p-1} - 3x_p}{x_p^2 - x_{p-1}^2}$

(c) $x_{p+1} = 4x_p - x_p^3 + 3x_{p-1} - x_p^2 x_{p-1}$

(d) $x_{p+1} = \frac{x_p^2 - 3}{x_p^2 - x_{p-1}^2}$