Technische Universität Graz
Institut für Theoretische Physik

COMPUTERMETHODEN DER TECHNISCHEN PHYSIK
Exam 1 WS 2021/2022

08.02.2022

This written exam for the lecture *Computational Methods in Technical Physics* consists of four 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. Solutions to the exercises can be submitted in the form of a scanned pdf or jpg file.

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 as an integral part of the examination.

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

Good luck!

1 Short questions (25 points)

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

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

(ii) **(5 points)** The matrix

$$A = \begin{bmatrix} 1 & 1 & 5 \\ 1 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix}$$

has three eigenvalues of distinct magnitude. Which of the following techniques can be used to determine all eigenvectors and eigenvalues of A? List all possibilities (multiple answers possible).

(a) Jacobi rotations

(b) The power method (von Mises iteration)

(c) QR decomposition

(d) Application of Gershgorin's theorem together with deflation

(iii) **(5 points)** Given a data set $y_i(x_i)$ for $i = 1 \ldots n$ with $n > m$. Minimizing the expression

$$\sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{m} a_j x_i^{j-1} \right)^2$$

with respect to the parameters a_j corresponds to

(a) a polynomial interpolation
(b) a polynomial fit
(c) a quadratic spline interpolation
(d) a nonlinear least-squares fit

(iv) **(5 points)** Consider the following statements:

- In numerical differential calculus, reducing the step size always improves the numerical accuracy.
- A polynomial interpolation of n data points requires solving a linear system of $n + 1$ equations.

Which of the following is true?

(a) Both statements are correct.
(b) The first statement is correct and the second is false.
(c) The first statement is false and the second is correct.
(d) Both statements are false.

(v) **(5 points)** Consider the following statements:

- The system of equations $x + y = 2.01$ and $y - 3x = -2.00$ is ill-conditioned.
- A discrete Fourier transform is equivalent to an interpolation with complex exponential functions.

Which of the following is true?

(a) Both statements are correct.
(b) The first statement is correct and the second is false.
(c) The first statement is false and the second is correct.
(d) Both statements are false.

2 A boundary value problem (25 points)

Consider the following boundary value problem for the function $y(x)$ on the one-dimensional domain $x = [x_1 \ldots x_N]$

$$\begin{aligned} y''' + ay'' &= 0 \\ y(x_1) &= \alpha_1 \\ y(x_N) &= \alpha_N \\ y'(x_N) &= \beta_N, \end{aligned} \tag{1}$$

with α_1, α_N and β_N being constants.

(i) **(5 points)** Reduce Eq. (1) to a set of first-order differential equations of the form $\boldsymbol{y}(x)' = f(\boldsymbol{y}(x), x)$.

(ii) **(5 points)** Write the boundary conditions in x_i in the form $g_{ij} = 0$, where j enumerates the boundary conditions.

We will solve the equation using a shooting algorithm, starting the integration from the initial condition $\boldsymbol{y}(x_1) = (\alpha_1, \beta_1, \gamma_1)$.

(iii) **(5 points)** Explain the steps of the shooting algorithm in words and formulate a convergence criterion in terms of a small parameter ε.

We perform the integration on an equidistantly spaced grid with step size h using a Runge-Kutta integration scheme given by

$$\begin{aligned} \boldsymbol{y}(x_i + h) &= \boldsymbol{y}(x_i) + f\big(\boldsymbol{Y}_2, x_i + \frac{h}{2}\big)h \\ \boldsymbol{Y}_2 &= \boldsymbol{y}(x_i) + f\big(\boldsymbol{Y}_1, x_i\big)\frac{h}{2} \\ \boldsymbol{Y}_1 &= \boldsymbol{y}(x_i). \end{aligned}$$

(iv) **(5 points)** Derive the equations for $\boldsymbol{Y}_1$, $\boldsymbol{Y}_2$ and $\boldsymbol{y}(x_i + h)$ from Eq. (1) in terms of $\boldsymbol{y}(x_i)$, a and h.

(v) **(5 points)** Perform a Taylor expansion of $\boldsymbol{y}(x)$ around x_i and show that the result is equivalent to the result obtained in part (iv).

3 Solving a system of linear equations (25 points)

Consider the system of linear equations

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

Using $\boldsymbol{x} = (v, w)$, Equation (2) can be rewritten as $A\boldsymbol{x} = LU\boldsymbol{x} = \boldsymbol{b}$, with L being a lower-diagonal matrix with ones on the diagonal, and U being upper-diagonal.

(i) **(5 points)** Calculate the matrices L and U.

(ii) **(5 points)** Explain how the LU decomposition can be used to solve Equation (2).

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

$$\boldsymbol{x}_{p+1} = B\boldsymbol{x}_p + \boldsymbol{c}. \tag{3}$$

(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)** The expression from part (iv) can be expressed as $\boldsymbol{x}_{p+1} = \boldsymbol{x}_p - \Delta\boldsymbol{x}_p$ where $\Delta\boldsymbol{x}_p$ is calculated using the Jacobi algorithm. Give the general expression for $\Delta\boldsymbol{x}_p$ in terms of the components of A and $\boldsymbol{b}$ and calculate $\Delta\boldsymbol{x}_p$ either from Eq. (2) or from part (iv).

*Hint: Inserting the solution $\boldsymbol{x}_{exact}$ into Equation (3) leads to a relation between $\boldsymbol{x}_{p+1} - \boldsymbol{x}_{exact}$ and $\boldsymbol{x}_p - \boldsymbol{x}_{exact}$.

4 Eigenvalues of a matrix (25 points)

The matrix

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

has one dominant eigenvalue. To find it, we start a power iteration with the vector $\boldsymbol{x}_0 = (1, 0, 0)$.

(i) **(5 points)** Show that the vector $\boldsymbol{x}_p$ (after p power iterations) is given by

$$\boldsymbol{x}_p = \lambda_1^p \left[c_1 \boldsymbol{v}_1 + c_2 \left(\frac{\lambda_2}{\lambda_1} \right)^p \boldsymbol{v}_2 + c_3 \left(\frac{\lambda_3}{\lambda_1} \right)^p \boldsymbol{v}_3 \right],$$

with λ_i and $\boldsymbol{v}_i$ being the eigenvalues and eigenvectors of A, respectively, and c_i being an unknown coefficient.

(ii) **(5 points)** Explain why the matrix A must have a single dominant eigenvalue for the power iteration to work.

(iii) **(5 points)** What are the elements of the vector $\boldsymbol{x}_3$ (after 3 power iterations, without normalizing the vector in between)?

(iv) **(5 points)** Explain how the largest eigenvalue can be estimated from the vectors $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$.

(v) **(5 points)** Given that the largest eigenvalue of A equals $\lambda_1 = 8$, calculate the error incurred by estimating the eigenvalue based on $\boldsymbol{x}_2$ and $\boldsymbol{x}_3$.