İzmir Kâtip Çelebi University
Department of Engineering Sciences

IKC-MH.55
Scientific Computing with Python
Take-home Final Examination

January 19, 2024 14:00 – January 24, 2024 23:59

Good Luck!

NAME-SURNAME:

SIGNATURE:

ID:

DEPARTMENT:

DURATION: Due to January 24, 2024

◇ **Answer at least 1 question from each parts and at most 4 questions.**
◇ **Prepare your report/codes.**
◇ **Copy your files into a directory named as your ID.**
◇ **Upload a single file by compressing this directory to UBYS.**

Question	Grade	Out of
1		25
2		25
3		25
4		25
TOTAL		

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Part I

Numerical Techniques: Differential Equations - Boundary Value & Eigenvalue Problems

Choose only two questions.

A) Compute the following boundary value problems with the boundary conditions given next to them, and Write a program that compares it to analytical solutions:

$$y'' - xy' + y = -x^2 \quad with \quad y(0) = -2, \; \& \quad y(1) = 1,$$
$$y'' = -(y')^2 - y + lnx \quad with \quad y(1) = 0, \quad \& \; y(2) = ln2$$

The analytical solutions of these equations are:

$$y(x) = 1 + 2\frac{e^{2x} - e^x}{e^2 - e}$$
$$y(x) = lnx$$

B) Write a program that solve the following eigenvalue problems with the given boundary conditions and find the smallest two eigenvalues:

$$y'' - 3y' + 2k^2 y = 0 \quad with \;\; y(0) = 0, \;\; y(1) = 0,$$
$$y'' + k^2 x^2 y = 0 \quad with \;\; y(0) = 0, \;\; y(1) = 0$$

C) **Pöschl-Teller potential** It is a widely used potential function used for matter diffusion in modern optoelectronic devices:

$$V(x) = -\frac{\hbar^2}{2m}\frac{\alpha^2}{cosh^2 \alpha x}$$

Where, α is a parameter that defines both the intensity and range of the potential together. It would be $\alpha = 0.05$ for typical devices. Take the constants in the Schrödinger equation $\hbar/2m = 7.62 \; eV\text{Å}^2$. Write a program to find the ground state energy by solving the Schrödinger equation with the boundary conditions $\psi(0) = \psi(100) = 0$ in the interval x : [0, 100 Å].

Part II

Numerical Techniques: Linear Algebra and Matrix Computing

Choose only one question.

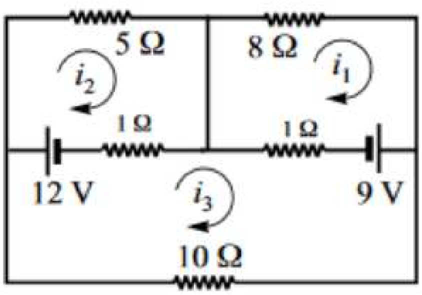
A) Write a program that solves the following systems of linear equations using Gaussian elimination:

$$\begin{aligned} x_1 + x_2 + x_4 &= 2 \\ 2x_1 + x_2 - x_3 + x_4 &= 1 \\ 4x_1 - x_2 - 2x_3 + 2x_4 &= 0 \\ 3x_1 - x_2 - x_3 + 2x_4 &= -3 \end{aligned} \qquad \begin{aligned} 4x_1 + 8x_2 + 4x_3 &= 8 \\ x_1 + 5x_2 + 4x_3 - 3x_4 &= -4 \\ x_1 + 4x_2 + 7x_3 + 2x_4 &= 10 \\ x_1 + 3x_2 - 2x_4 &= -4 \end{aligned}$$

B) Write a program that first checks that the determinants of the matrices given below are as being nonzero and then calculates their inverses. (There is a simple way to check your results: Multiply each matrix by its inverse and it should result as a unit matrix.)

$$\begin{pmatrix} 3 & 2 & -1 \\ 0 & -1 & 4 \\ 6 & 3 & 2 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 & -2 & 3 \\ 3 & 1 & 1 & 4 \\ -1 & 0 & 2 & -1 \\ 4 & 3 & 6 & 0 \end{pmatrix}$$

C) Set up a system of equations that give the currents with Kirchhoff's rules for the direct current circuit given in the figure and write a program that calculates these currents.



Part III

Data Analysis: Interpolation and Curve Fitting

Choose only one question.

A) Bessel functions cannot be expressed in terms of known functions, but are defined as a series of infinite terms as follows:

$$J_n(x) = \sum_{k=0}^{\infty} = \frac{(-1)^k}{k!(n+k)!} \left(\frac{x}{2}\right)^{n+2k}$$

The values of $J_0(x)$ in the range of [0,3] are given in the table below:

x	$J_0(x)$
0.0	1.00000000
0.5	0.93846981
1.0	0.76519769
1.5	0.51182767
2.0	0.22389078
2.5	−0.04838378
3.0	−0.26005195

Write a python program that establishes the Lagrange interpolation for Bessel functions at these 7 points and interpolate at $x = 1.75$ and $x = 2.99$, then compare them with their exact values ($J_0(1.75) = 0.36903253$ ve $J_0(2.99) = -0.25664274$). Which value would be more inaccurate? Explain.

B) The volume variation of a liquid with the temperature is given in the table below:

V (cm^3)	T (°C)
1.032	10.0
1.094	29.5
1.156	50.0
1.215	69.5
1.273	90.0

Write a python program to find the coefficients a and b by assuming that this liquid volume varies with the relation $V = 1 + aT + bT^2$.

C) For the given data points;

x	Y
0.000	1.500
0.142	1.495
0.285	1.040
0.428	0.821
0.571	1.003
0.714	0.821
0.857	0.442
1.000	0.552

to which we will fit $y(x) = \alpha e^{\beta x}$.

- First, we should compute a new table with $z(x) = lny(x)$
- Construct the normal equations for $z = A + Cx$ where $A = ln\alpha$ and $C = \beta$
- Solve these normal equations to find A and C
- Convert back to the original variables
- Plot Y vs x and y vs x then compare them.