Advanced Numerical Analysis for Chemical Engineering
Final Examination -1 (3 hrs.)

Instruction: *Closed book and closed notes examination.*

1. (a) State True of False. Justify your answer.

   1. There exists a 4×4 matrix whose row space contains $\begin{bmatrix} 1 & 2 & 1 & 1 \end{bmatrix}^T$ and whose null space contains $\begin{bmatrix} 1 & -2 & 1 & 1 \end{bmatrix}^T$. (2 marks)
   2. The rank of a $n \times n$ matrix with every $a_{ij} = c$ where c is a constant is one. (2 marks)

   (b) Consider matrix

$$\mathbf{B} = \begin{bmatrix} 1 & 2 & -1 \\ -1 & -2 & 1 \\ 1 & 2 & -1 \end{bmatrix}$$

   1. What is rank of matrix B? Find a basis for the **left null space** of matrix **B** (i.e. null space of $\mathbf{B}^T$). (4 marks)
   2. Find projection of vector $\mathbf{b} = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}^T$ into the row space of matrix **B**. (4 marks)

   (c) Consider an $n \times n$ positive symmetric definite matrix **A**. Matrix A can be expressed as

$$\mathbf{A} = \mathbf{\Psi \Lambda \Psi}^T$$

   where $\mathbf{\Psi}$ is the matrix containing orthonormal eigen vectors of **A** and $\mathbf{\Lambda}$ is a diagonal matrix with eigen values of A appearing on it's diagonal. Show that the condition number of matrix $\mathbf{\Psi}$ is 1, i.e. $C(\mathbf{\Psi}) = \mathbf{1}$. (4 marks)

   (d) Prove the following inequalities

$$\|\mathbf{AB}\| \leq \|\mathbf{A}\| \, \|\mathbf{B}\|$$

$$C(\mathbf{AB}) \leq C(\mathbf{A})C(\mathbf{B})$$

   for arbitrary matrices **A** and **B** where $C(.)$ represents the condition number. (4 marks)

2. **Optimization and parameter estimation**

   (a) An objective function (cost) for design of a 50 stage distillation column is given as

$$\phi(P, R) = 14720(100 - P) + 6560R - 30PR - 6560 - 30P$$

   Using the necessary conditions for optimality, find optimum values of reflux ratio (R) and % recovery in bottom stream (P) that minimize the cost $\phi(P, R)$. (4 marks)

   (b) Table (1) presents data for distribution of SO_3 in Hexane. It is desired to fit following model to data

$$\mathbf{y} = \boldsymbol{\alpha} \mathbf{P}^{\beta}$$

   Calculate least square estimates of model parameters (α, β) by suitably transforming the model and using linear least square method.. (5 marks)

Run No.	P pressure (psia)	y (wt.fr.of Hexane)
1	200	0.85
2	400	0.57
3	600	0.40
4	1200	0.21
5	1600	0.08

Table 1: Reaction Rate Data

(c) Suppose it is desired to estimate the model parameters using the Gauss-Newton method. Perform one iteration of Gauss-Newton step using estimates of (α, β) generated in part (a). (5 marks)

3. **ODE-IVP and ODE-BVP**

(a) Progress of a chemical reaction in a batch reactor is described by the following set of ODE-IVP

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x} \quad ; \quad \mathbf{x}(\mathbf{0}) = \begin{bmatrix} 1 & 1 \end{bmatrix}^T$$
$$\mathbf{A} = \begin{bmatrix} -3 & -1 \\ -1 & -3 \end{bmatrix}$$

where $\mathbf{x}(t)$ represents vector of reactor concentrations.

1. Find solution $\mathbf{x}(t) = \exp(At)\mathbf{x}(\mathbf{0})$ using eigen values and eigen vectors of $\mathbf{A}$. (3 marks)
2. Comment upon qualitative behavior of solutions based on eigen values of matrix $\mathbf{A}$. ((2 marks)

(b) The steady state behavior of an isothermal tubular reactor with axial mixing, in which a first order irreversible reaction is carried out, is represented by following ODE-BVP

$$\frac{d^2C}{dz^2} - \frac{dC}{dz} - 6C = 0$$
$$At\ z = 0 : \frac{dC}{dz} = C(0) - 1 \ ; \ At\ z = 1 : \frac{dC}{dz} = 0$$

It is desired to solve this problem using the method of orthogonal collocations.

1. For the choice of internal collocation points at $z = 0.2$ and $z = 0.8$, write down the appropriate algebraic equations to be solved in terms of unknowns. The $\mathbf{S}$ and $\mathbf{T}$ matrices for the given choice of roots are listed below. (4 marks).

$$\mathbf{S} = \begin{bmatrix} -7 & 8.2 & -2.2 & 1 \\ -2.7 & 1.7 & 1.7 & -0.7 \\ 0.7 & -1.7 & -1.7 & 2.7 \\ -1 & 2.2 & -8.2 & 7 \end{bmatrix} \quad ; \quad \mathbf{T} = \begin{bmatrix} 24 & -37.2 & 25.2 & -12 \\ 16.4 & -24 & 12 & -4.4 \\ -4.4 & 12 & -24 & 16.4 \\ -12 & 25.2 & -37.2 & 24 \end{bmatrix}$$

2. Rearrange the equations derived in above the standard form $\mathbf{Ax} = \mathbf{b}$ where

$$\begin{aligned} \mathbf{x} &= \begin{bmatrix} C_0 & C_1 & C_2 & C_2 \end{bmatrix}^T \\ C_0 &\equiv C(0), \quad C_1 \equiv C(0.2), \quad C_2 \equiv C(0.8), \quad C_3 \equiv C(1) \end{aligned}$$

Is matrix $\mathbf{A}$ diagonally dominant? Suppose it is desired to solve $\mathbf{Ax} = \mathbf{b}$ using Gauss-Seidel method. Can you arrive at any conclusion regarding the convergence of Gauss-Seidel method only based on the diagonal dominance of $\mathbf{A}$? (3 marks)

(c) It is desired to solve the following scalar ODE-IVP

$$\frac{dx}{dt} = f(x,t) \;\; ; \quad x(t_n) = x(n)$$

using following multi-step algorithm.

$$x(n+1) = \alpha_0 x(n) + \alpha_1 x(n-1) + h\left[\beta_0 f(n) + \beta_{-1} f(n+1)\right]$$

using local polynomial approximation of the form

$$x^{(n)}(t) = a_{0,n} + a_{1,n} t + a_{2,n} t^2 + a_{3,n} t^3$$

Find the coefficients $(\alpha_0, \alpha_1, \beta_0, \beta_{-1})$ and state the final form of the integration algorithm. (4 marks)

Note: The exactness constraints are given as

$$\begin{aligned} \sum_{i=0}^{p} \alpha_i &= 1; \qquad (j=0) \\ \sum_{i=0}^{p} (-i)^j \alpha_i + j \sum_{i=-1}^{p} (-i)^{j-1} \beta_i &= 1 \;\; ; \quad (j = 1, 2, ..., m) \end{aligned}$$

$$\text{Note} : (i)^j = 1 \;\text{ when }\; i = j = 0$$