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

Instruction: Closed book and closed notes examination.

1. (a) State True or False. Justify your answer.
   1. There exists a $4 \times 4$ matrix whose row space contains $[1 \ 2 \ 1 \ 1]^T$ and whose null space contains $[1 \ -2 \ 1 \ 1]^T$. (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

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

1. What is rank of matrix $B$? Find a basis for the left null space of matrix $B$ (i.e. null space of $B^T$). (4 marks)
2. Find projection of vector $b = [1 \ 1 \ 1]^T$ 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

$$A = \Psi \Lambda \Psi^T$$

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

(d) Prove the following inequalities

$$\|AB\| \leq \|A\| \|B\|$$

$$C(AB) \leq C(A)C(B)$$

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

$$y = \alpha P^\beta$$

Calculate least square estimates of model parameters ($\alpha, \beta$) by suitably transforming the model and using linear least square method. (5 marks)
<table>
<thead>
<tr>
<th>Run No.</th>
<th>( P ) pressure (psia)</th>
<th>( y ) (wt.fr.of Hexane)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>200</td>
<td>0.85</td>
</tr>
<tr>
<td>2</td>
<td>400</td>
<td>0.57</td>
</tr>
<tr>
<td>3</td>
<td>600</td>
<td>0.40</td>
</tr>
<tr>
<td>4</td>
<td>1200</td>
<td>0.21</td>
</tr>
<tr>
<td>5</td>
<td>1600</td>
<td>0.08</td>
</tr>
</tbody>
</table>

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 \((\alpha, \beta)\) 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

\[
\frac{dx}{dt} = Ax \quad ; \quad x(0) = \begin{bmatrix} 1 & 1 \end{bmatrix}^T
\]

where \( x(t) \) represents vector of reactor concentrations.

1. Find solution \( x(t) = \exp(At)x(0) \) using eigen values and eigen vectors of \( A \). (3 marks)
2. Comment upon qualitative behavior of solutions based on eigen values of matrix \( A \). (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 \( S \) and \( T \) matrices for the given choice of roots are listed below. (4 marks).

\[
S = \begin{bmatrix}
-7 & 8.2 & -2.2 & 1 \\
-2.7 & 1.7 & 1.7 & -0.7 \\
0.7 & -1.7 & -1.7 & 2.7 \\
-1 & 2.2 & -8.2 & 7
\end{bmatrix} \quad ; \quad T = \begin{bmatrix}
24 & -37.2 & 25.2 & -12 \\
16.4 & -24 & 12 & -4.4 \\
-4.4 & 12 & -24 & 16.4 \\
-12 & 25.2 & -37.2 & 24
\end{bmatrix}
\]
2. Rearrange the equations derived in above the standard form \( Ax = b \) where

\[
\begin{bmatrix}
    x_0 & C_1 & C_2 & C_2
\end{bmatrix}^T
\]

\( C_0 \equiv C(0), \quad C_1 \equiv C(0.2), \quad C_2 \equiv C(0.8), \quad C_3 \equiv C(1) \)

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

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

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

using following multi-step algorithm.

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

using local polynomial approximation of the form

\[
x^{(\alpha)}(t) = a_{0,n} + a_{1,n}t + a_{2,n}t^2 + a_{3,n}t^3
\]

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

\[
\sum_{i=0}^{p} \alpha_i = 1; \quad (j = 0)
\]

\[
\sum_{i=0}^{p} (-i)^j \alpha_i + j \sum_{i=-1}^{p} (-i)^{j-1} \beta_i = 1; \quad (j = 1, 2, \ldots, m)
\]

Note: \((i)^j = 1\) when \(i = j = 0\)