Run No.	$\mathbf{r}_R$	C_A	C_R
1	1.25	2	8
2	2.5	4	6
3	4.1	6	4
4	0.75	1.5	8.5
5	3.5	5	5

Table 1: Reaction Rate Data

Advanced Numerical Analysis for Chemical Engineering
Final Examination -2 (3 hrs.)

Instruction: *Closed book and closed notes examination.*

1. (a) For a general 2×2 matrix

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

which iterative scheme, Jacobi or Gauss -Seidel, will converge faster? (4 marks)

(b) It is desired to optimize the following objective function with respect vector $\mathbf{x}$.

$$f(\mathbf{x}) = x_1 - x_2 + 2(x_1)^2 + 2x_1x_2 + (x_2)^2$$

Use the necessary conditions for optimality to compute the optimum and comment upon whether the stationary point is a maximum or a minimum. (4 marks)

(c) Consider matrix

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

Find a basis for the null space of matrix $\mathbf{B}$. Also, find projection matrix $\mathbf{P}_r$ that projects any vector from R^3 into the null space of matrix $\mathbf{B}$. (5 marks)

(d) Prove the following inequality giving the lower bound on the numerical error in solution of linear algebraic equations $\mathbf{Ax} = \mathbf{b}$

$$\frac{\|\delta \mathbf{x}\|}{\|\mathbf{x}\|} \geq \frac{1}{C(\mathbf{A})} \frac{\|\delta \mathbf{b}\|}{\|\mathbf{b}\|}$$

where $C(\mathbf{A})$ represents condition number of matrix $\mathbf{A}$. (3 marks)

2. Table 1 presents rate data for reaction $A \leftrightarrow R$. It is desired to fit following two models to this rate data

- Model A: Irreversible first order reaction model

$$\mathbf{r}_R = k_0 C_A$$

- Model B: Reversible first order reaction model

$$\mathbf{r}_R = k_1 C_A - k_2 C_R$$

(a) Calculate least square estimates of both the reaction rate expressions using data given in Table 1. (5 marks)

(b) Estimate covariance of estimated model parameters in each case. (4 marks)

(c) Compare the two models based on correlation coefficient ($\mathbf{R}^2$) defined as

$$\mathbf{R}^2 = \frac{\mathbf{Y}^T \widehat{\mathbf{Y}}}{\mathbf{Y}^T \mathbf{Y}}$$

where $\mathbf{Y} = \begin{bmatrix} (\mathbf{r}_R)_1 & (\mathbf{r}_R)_2 & ... & (\mathbf{r}_R)_5 \end{bmatrix}^T$ and $\widehat{\mathbf{Y}} = \begin{bmatrix} (\widehat{\mathbf{r}}_R)_1 & (\widehat{\mathbf{r}}_R)_2 & ... & (\widehat{\mathbf{r}}_R)_5 \end{bmatrix}^T = \mathbf{\Phi}\widehat{\boldsymbol{\theta}}$. Here, $(\widehat{\mathbf{r}}_R)_i$ indicates estimated value of reaction rate using least square estimates of model parameters. Which model fits better? (Note: Higher the value of $\mathbf{R}^2$, better is the fit.) (3 marks)

(a) 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

$$\frac{d^2C}{dz^2} - \frac{dC}{dz} - 6C = 0$$

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

1. Represent the above second order equation in the standard form $d\mathbf{x}/dz = \mathbf{Ax}$ by appropriately defining a state vector $\mathbf{x}$. Compute $exp(\mathbf{A}z)$ using eigen values and eigen vectors of matrix $\mathbf{A}$. (4 marks)
2. Find the missing initial condition at $z = 0$ such that the analytical solution

$$\mathbf{x}(z) = exp(\mathbf{A}z)\mathbf{x}(0)$$

satisfies the boundary condition at $z = 1$. (4 marks)

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

$$\frac{dx}{dt} = f(x,t) \ ; \ \ x(t_n) = x(n) \tag{1}$$

using Milne's multi-step algorithm. The Milne's implicit formulae for solving ODE-IVPs are obtained by imposing following additional constraints

$$\alpha_0 = \alpha_2 = \alpha_3 = ... = \alpha_p = 0 \text{ and } \alpha_1 \neq 0$$

along with the exactness constraints and selecting $p = m - 2$. Find the coefficients of the 3'rd order Milne's implicit algorithm (i.e. $m = 3$, $p = 1$) and state the final form of the integration algorithm. (4 marks)

Note: The exactness constraints are given as

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

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

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

(c) Consider the ODE-IVP given by equation (1). We know value $x(n)$ at $t = t_n$ and we wish to integrate the equation to obtain $x(n+1)$ at $t = t_{n+1} = t_n + h$ using *orthogonal collocation* method with two internal collocation points lying between $[t_n, t_{n+1}]$. (Here, h represents fixed integration step size).

1. Transform the ODE-IVP in terms of an independent variable τ such that $\tau = 0$ corresponds to $t = t_n$ and $\tau = 1$ corresponds to $t = t_{n+1} = t_n + h$. (1 marks)
2. For the choice of internal collocation points at $\tau = 0.2$ and $\tau = 0.8$, write down the appropriate algebraic equations to be solved in terms of unknowns $x(0.2)$, $x(0.8)$ and $x(1)$ by setting residuals to zero at internal collocation points and at $\tau = 1$. (5 marks)
3. Arrange the resulting set of equation in the following form

$$A\mathbf{z} = \mathbf{F}(\mathbf{z})$$

where $\mathbf{z} = \begin{bmatrix} x(0.2) & x(0.8) & x(1) \end{bmatrix}^T$ and how the resulting set of nonlinear equations can be solved by Gauss-Seidel type successive substitution scheme. (4 marks)

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