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

Q1.(a) Given the measurements $b_1, ..., b_n$ at distant points $t_1, ..., t_n$. Show that the straight line

$$b = C + Dt \ + e$$

which minimizes $\sum e^2$ comes from the least squares:

$$\begin{bmatrix} n & \sum t_i \\ \sum t_i & (\sum t_i)^2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \sum b \\ \sum b_i t_i \end{bmatrix}$$

(3 marks)

(b) Find the best staright line fit to the following measurements (3 marks)

$$\begin{aligned} y &= 2 \ at \ t = -1 \ ; \ y = 0 \ at \ t = 0 \\ y &= -3 \ at \ t = -1 \ ; \ y = -5 \ at \ t = 2 \end{aligned}$$

(c) Find a vector x orthogonal to row space, and a vector y orthogonal to column space, of (2 marks)

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 3 \\ 3 & 6 & 4 \end{bmatrix}$$

(d) It is desired to minimize the following objective function

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

(i) analytically and (ii) using Newton's method starting from $x^{(0)} = [0 \ 0]^T$. Perform one iteration by Newton's method assuming step length parameter $\lambda = 1$ (Do not perform one dimensional optimization). How close is $\begin{bmatrix} x_1^{(1)} & x_2^{(1)} \end{bmatrix}$ generated by Newton's method to the stationary point of $\Phi(\mathbf{x})$? Is the stationary point of $\Phi(\mathbf{x})$ a maximum or a minimum ?
marks)

Q2. (a) For a general 2×2 matrix

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

which iterative scheme, Jacobi or Gauss -Seidel, will cobverge faster? (6 marks)

(b) It is desired to apply the method of finite difference to solve the following PDE

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial z^2}$$

$$\begin{aligned} \text{Boundary Conditions} &: \quad C(0,t) = C(1,t) = 0 \\ \text{Initial Condition} &: \quad C(z,0) = 1 \end{aligned}$$

where t and z represent dimensionless time and dimensionless length, respectively.

(i)Assuming 'n' equidistant grid points, obtain a set of ODE-IVP from the PDE and arrange these equations in a standard form $d\mathbf{x}/dt = A\mathbf{x}$. marks)

(ii) Suppose the resulting set of ODE-IVP is to be integrated using implicit Euler method. Find the condition on the integration step size 'h' in terms of eigenvalues of matrix A so that the approximation error will decay exponentially and approximate solution will approach the true solution. The eigenvalues of matrix A are given by

$$\lambda_i = -4\sin^2\left[\frac{\pi i}{2(n+1)}\right] \quad ; \quad i = 1, 2, ...n$$

(4 marks)

Q3. (a) Consider the following system

$$\begin{aligned} dy_1/dt &= -y_1 \\ dy_2/dt &= y_1 - 2y_2 \\ dy_3/dt &= -y_1 + y_2 - 3y_3 \\ y_1(0) &= 2; \quad y_2(0) = 1 \;\; ; \;\; y_3(0) = 2 \end{aligned}$$

(a) Compute the analytical solution to ODE-IVP using eigenvalue and eigenvector based method. and calculate the stiffness ratiofor the system. (6 marks)

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

$$\frac{dx}{dt} = f(x,t) \;\; ; \quad x(0) = x_0$$

using a multi-step algorithm of the form $t = 0$

$$x(n+1) = \sum_{i=0}^{p} \alpha_i x(n-i) + h \sum_{i=-1}^{p} \beta_i \ f(n-i)$$

where $x(n-i) = x(t_{n-i})$; $f(n-i) = f(x(t_{n-i}), t_{n-i})$ and h is the integration step size. The Adam's Moulton implicit formulae for solving the ODE-IVP is obtained by imposing the following additional constraints along with the exactness constraints for order 'm' algorithm

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

Show that, in order to solve for $\{\alpha_i\}$ and $\{\beta_i\}$ exactly in this case, p should be selected as $p = m - 2$. also, obtain the coefficients for 3'rd order Adam's Moulton's implicit algorithm (i.e. $m = 3, p = 1$). (6 marks)

Q4. (a) Very common model for a dimensionless first-order chemical reaction is

$$dC/dt = -kC$$

The integrated form of this model is $C = C(0)\exp(-kt)$, which is non linear in the parameter k and initial concentration $C(0)$. .

t	0.2	0.5	1	1.5	2
C	0.75	0.55	0.21	0.13	0.04

We do not have a measurement of the initial concentration at $t = 0$ and it is desired to estimate both $C(0)$ and k using the data given above. First transform the original model to a linear in parameter form and estimate the model parameters. (5 marks)

(b) Perform one iteration by Gauss-Newton method starting from solution of part (a) as initial guess. (5 marks)