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

1. Consider matrix

$$M = \begin{bmatrix} 1 & 2 & 5 \\ -2 & -1 & -4 \\ -1 & -2 & -5 \\ 0 & 1 & 2 \\ 2 & 0 & 2 \end{bmatrix}$$

   (a) Find a basis for column space and for null space of M. (3 marks)

   (b) Project vector $\mathbf{b} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \end{bmatrix}^T$ onto the column space of matrix M. Also, find component of $\mathbf{b}$ in left null space of M. (5 marks)

   (c) Does the set of functions of the form

$$f(t) = a + bt$$

   ,where a and b are nonzero real constants, constitute a linear vector space? Here set of scalars is real line and $t \in [0, 1]$. (3 marks)

   (d) Consider application of finite difference method to solving ODE-BVP with non-equidistant grid point i.e.

$$\Delta z_i = z_{i+1} - z_i \;\; ; i = 0, 1, 2, ...$$

   Derive expressions for approximating the second derivatives (3 marks)

$$y_i^{(2)} = \frac{2}{\Delta z_i + \Delta z_{i-1}} \left[\frac{y_{i+1} - y_i}{\Delta z_i} - \frac{y_i - y_{i-1}}{\Delta z_{i-1}} \right] - \frac{1}{3} y_i^{(3)} \left(\Delta z_i - \Delta z_{i-1} \right) + ...$$

2. It is desired to fit the data given in the table below

r (rate)	C	T
1	0.8	4
7.5	0.8	5
0.7	0.4	4
5	0.4	5

   a nonlinear reaction rate equation of the form

$$r = K \frac{2C}{2 + C} \exp(-A/T)$$

   (Note that, to simplify numerical the calculations, scaled values of temperature variable are given in the above table).

   (a) Rearranging the model as

$$\ln \left[\frac{r(2 + C)}{2C} \right] = \ln (K) - \frac{A}{T}$$

   determine the parameters A and K using linear least square estimation. (5 marks)

(b) Estimate the covariance matrix of the parameters estimated in part (a), i.e., $\widehat{\boldsymbol{\theta}} = \begin{bmatrix} \ln(K) & A \end{bmatrix}$. (4 marks)

(c) Suppose, instead of using linearizing transformation given above, it is desired to estimate model parameters using Gauss-Newton method. Perform one iteration of Gauss-Newton starting of the estimate of A and K generated in part (a). (5 marks)

3. It is desired to apply the method of finite difference to solve the following PDE

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

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

where t and z represent dimensionless time and dimensionless length, respectively. Assuming 'n' equidistant grid points and defining vector

$$\mathbf{x} = \begin{bmatrix} C_1 & C_2 & ... & C_n \end{bmatrix}^T$$

we obtain the following set of ODE-IVP from the PDE

$$d\mathbf{x}/dt = A\mathbf{x} \ ; \ \mathbf{x}(0) = \begin{bmatrix} 1 & 1 & ... & 1 \end{bmatrix}^T$$

$$A = \frac{1}{(\Delta z)^2} \begin{bmatrix} -2 & 1 & 0 & .... & 0 \\ 1 & -2 & 1 & .... & 0 \\ .... & .... & .... & .... & .... \\ 0 & .... & 1 & -2 & 1 \\ 0 & .... & 0 & 1 & -2 \end{bmatrix}$$

(a) Suppose that it is desired to solve the resulting linear algebraic equations analytically as $\mathbf{x}(t) = [\Psi \exp(\Lambda t) \Psi^{-1}]\, \mathbf{x}(0)$ where $A = \Psi \Lambda \Psi^{-1}$. Show that vector

$$\mathbf{v}^{(k)} = \begin{bmatrix} \sin(k\pi\Delta z) & \sin(2k\pi\Delta z) & ..... & \sin(nk\pi\Delta z) \end{bmatrix}^T$$

is an eigenvector of matrix A with eigenvalue

$$\lambda_k = \frac{2}{(\Delta z)^2} \left[\cos(k\pi\Delta z) - 1 \right]$$

where and $k = 1, 2, ...n$ and $\Delta z = 1/(n+1)$. (Show calculations for 1^{st}, i^{th} and the last row). (5 marks).

(b) Comment upon the asymptotic behavior of the resulting solution as $t \to \infty$. (Justify your comments). (4 marks).

(c) Suppose, instead of solving the problem analytically, the set of ODE-IVP is to be integrated using Crank-Nicholson method (i.e. trapezoidal rule). 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. (5 marks).

Note: Crank-Nicholson algorithm for the scalar case can be stated as

$$x(n+1) = x(n) + \frac{h}{2}\left[f(n) + f(n+1)\right]$$

(d) It is desired to derive 3'rd order Gear's implicit integration formula of the form

$$x(n+1) = \alpha_0 x(n) + \alpha_1 x(n-1) + \alpha_2 x(n-2) + h\beta_{-1} f(n+1)$$

for numerically integrating an ODE-IVP of the form

$$dx/dt = f(x,t) \quad ; \quad I.c. : x(t_n) = x(n) \tag{1}$$

from $t = t_n$ to $t = t_n + 1$. Setup the necessary constraint equations and obtain coefficients $\{\alpha_i\}$ and β_{-1}. (4 marks)

Note: The exactness constraints are given as

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

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

(e) A chemical reactor is modelled using the following set of ODE-IVP

$$\frac{dC}{dt} = \frac{1-C}{V} - 2C^2 \tag{2}$$

$$\frac{dV}{dt} = 1 - V \tag{3}$$

Linearize the above equations in the neighborhood of steady state $C = 0.5$ and $V = 1$ and develop a linear perturbation model. Obtain the analytical solution for the linearized system starting from initial condition $C = 0.7$ and $V = 0.8$. Also, compute stiffness ratio and comment upon asymptotic stability of the solution. (4 marks)