Advanced Numerical Analysis for Chemical Engineering
Mid-Term Examination (2 hrs.)

1. Tube side output temperature measurements, $\begin{pmatrix} T_1 & T_2 & .... & T_n \end{pmatrix}$, have been collected from a shell and tube heat exchanger system operating at a steady state operating point. It is desired to fit a model of the form

$$T_i = \beta + e_i$$

using this data where constant β is an unknown parameter and e_i represents the approximation error.

   (a) Show that the least square estimate of parameter β can be obtained by projecting vector $\mathbf{U}$

$$\mathbf{U} = \begin{bmatrix} T_1 & T_2 & .... & T_n \end{bmatrix}^T$$

   on vector

$$\mathbf{a} = \begin{bmatrix} 1 & 1 & .... & 1 \end{bmatrix}^T$$

   Also, show that the least square estimate of β correspond to the mean of the temperature data. (2 marks)

   (b) The horizontal line $T = 3$ is closest to vector $\mathbf{U} = \begin{bmatrix} 1 & 2 & 6 \end{bmatrix}^T$. Check that the vector

$$\mathbf{p} = \begin{bmatrix} 3 & 3 & 3 \end{bmatrix}^T$$

   is perpendicular to error vector, $\mathbf{e} = \mathbf{U} - \mathbf{p}$, and find the projection matrix $\mathbf{P}_r = A\left(A^T A\right)^{-1} A^T$, which generates the projection vector $\mathbf{p}$ from vector $\mathbf{U}$. Also, state what is rank of the projection matrix $\mathbf{P}_r$. (3 marks)

2. Relative height of a terrain (in meters) is measured at four corners (1,0), (0,1), (-1,0) and (0,-1) of a square field and was found to be 0, 1, 3, and 4 meters, respectively. Find the plane that gives best fit to four points in the least square sense. The equation for the plane is given as follows

$$h = \alpha + \beta x + \delta y$$

In other words, find the least square estimates of parameters (α, β, δ) using the given data. Also, show that, at the center of the square, we have $\widehat{h} = \widehat{\alpha} + \widehat{\beta} x + \widehat{\delta} y =$ mean of heights at the four corners. (6 marks)

3. Consider the following coupled differential equations characterize a system

$$\begin{aligned} \frac{d^2u}{dz^2} - u\frac{dv}{dz} &= 5u\sin(v) \quad for\ \ 0 < z < 1 \\ \frac{d^2v}{dz^2} + v\frac{du}{dz} &= uv^2 \quad for\ \ 0 < z < 1 \end{aligned}$$

together with following boundary conditions

$$\begin{aligned} z &= 0 : \ u(0) = 0 \ \text{and}\, v(0) = 1; \\ z &= 1 : \ du\,(1)/dz = 0 \ \text{and}\, dv(1)/dz = 2(v(1) - 10) \end{aligned}$$

Obtain a set of nonlinear algebraic equations using orthogonal collocation with 2 collocation points and arrange them in generic form $F(\mathbf{x}) = \overline{0}$. What is vector $\mathbf{x}$ in this case? (6 marks)

Note: The collocation points are at $z_1 = 0.21$ and $z_2 = 0.79$ and the corresponding $\mathbf{S}$ and $\mathbf{T}$ matrices are as follows

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

4. Find an approximate solution of ODE-BVP

$$\frac{d^2u}{dz^2} + zu = 1$$

$$B.C.: u(0) = u(1) = 0$$

using Gelarkin's method and following form of the approximate solution

$$\widehat{u}(z) = az(1-z) + bz^2(1-z)$$

(8 marks)

Note: *(a) Inner product is defined as*

$$\langle f(z), g(z) \rangle = \int_0^1 f(z)g(z)dz$$

(b) Gelarkin's Method: Given approximate solution as linear combination of basis functions

$$\left\{ \widehat{u}^{(1)}(z), \widehat{u}^{(2)}(z), ..., \widehat{u}^{(m)}(z) \right\}$$

solve for the following set of m algebraic equations simultaneously

$$\left\langle \widehat{u}^{(i)}(z), \mathbf{L}\widehat{u}(z) - f(z) \right\rangle = 0 \quad \text{for } i = 1, 2, ...m$$