National University of Singapore
Ph.D. Qualifying Examination
Computational Mathematics, August 2024
Duration: 3h

Part I: Scientific Computing

Question 1 [17 marks]

Consider the $n \times n$ matrix

$$A = \begin{pmatrix} 2 & -1 & & & & -1 \\ -1 & 2 & -1 & & & \\ & -1 & \ddots & \ddots & & \\ & & \ddots & \ddots & -1 & \\ & & & -1 & 2 & -1 \\ -1 & & & & -1 & 2 \end{pmatrix}.$$

a) Show that for any vector $\mathbf{b} = (b_1, \cdots, b_n)^T$ satisfying $b_1 + \cdots + b_n = 0$, the linear system $A\mathbf{x} = \mathbf{b}$ has a one-dimensional solution space.

b) Show that the Jacobi method converges for the linear system $A\mathbf{x} = \mathbf{b}$. Describe which solution in the solution space the Jacobi method converges to.

Question 2 [16 marks]

Define the following points

- $\mathbf{x}_1 = (0, 0)^T$,
- $\mathbf{x}_2 = (1, 0)^T$,
- $\mathbf{x}_3 = (2, 0)^T$,
- $\mathbf{x}_4 = (0, 1)^T$,
- $\mathbf{x}_5 = (1, 1)^T$,
- $\mathbf{x}_6 = (2, 1)^T$,
- $\mathbf{x}_7 = (0, 2)^T$,
- $\mathbf{x}_8 = (1, 2)^T$,
- $\mathbf{x}_9 = (2, 2)^T$.

Let Ω_1 be the square with vertices $\mathbf{x}_1$, $\mathbf{x}_3$, $\mathbf{x}_7$, and $\mathbf{x}_9$. Let Ω_2 be the convex hull of $\mathbf{x}_1$, $\mathbf{x}_3$, $\mathbf{x}_6$, $\mathbf{x}_8$, and $\mathbf{x}_9$.

a) Find polynomials $p_1, \cdots, p_9$ such that $p_k(\mathbf{x}_j) = \delta_{jk}$ for all $j, k = 1, \cdots, 9$, and

$$\int_{\Omega_1} u(\mathbf{x})\,\mathrm{d}\mathbf{x} = \sum_{k=1}^{9} u(\mathbf{x}_k) \int_{\Omega_1} p_k(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

for all monomials $u(x, y) = x^m y^n$ with $0 \leqslant m \leqslant 2$ and $0 \leqslant n \leqslant 2$.

b) Find polynomials $q_1, \cdots, q_8$ such that $q_k(\mathbf{x}_j) = \delta_{jk}$ for all $j, k = 1, \cdots, 8$, and

$$\int_{\Omega_2} u(\mathbf{x})\,\mathrm{d}\mathbf{x} = \sum_{k=1}^{8} u(\mathbf{x}_k) \int_{\Omega_1} q_k(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

for all monomials $u(x,y) = x^m y^n$ with $0 \leqslant m \leqslant 2$, $0 \leqslant n \leqslant 2$, and $m + n \leqslant 3$.

Question 3 [16 marks]

Consider the Runge-Kutta method with the following Butcher's tableau:

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ c_1 & a_{21} & a_{22} & 0 \\ 1 & a_{31} & a_{32} & 0 \\ \hline & b_1 & b_2 & b_3 \end{array}$$

Find the values of a_{21}, a_{22}, a_{31}, a_{32}, c_1, b_1, b_2, b_3 such that the corresponding Runge-Kutta method has convergence order 4.

Question 4 [16 marks]

Consider the one-dimensional convection-diffusion equation

$$\begin{aligned} &\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \kappa \frac{\partial^2 u}{\partial x^2}, \qquad x \in \mathbb{R}, \quad t \in (0, +\infty), \\ &u(x,0) = u_0(x), \qquad x \in \mathbb{R}, \end{aligned}$$

where a and κ are constants, and $\kappa > 0$. We discretize the equation on a uniform spatial grid $\{x_j\}_{j\in\mathbb{Z}}$, where $x_{j+1} - x_j = \Delta x$ for any j; and the time steps are given by $0 = t_0 < t_1 < t_2 < \cdots$. Let U_j^n be the numerical approximation of

$$\frac{1}{\Delta x} \int_{x_j - \Delta x/2}^{x_j + \Delta x/2} u(x, t_n)\,\mathrm{d}x.$$

a) Suppose the function $v(x)$ satisfies the ordinary differential equation

$$\begin{aligned} &a v'(x) = \kappa v''(x), \\ &v(x_j) = U_j, \quad v(x_{j+1}) = U_{j+1}. \end{aligned}$$

Find the value of $F(U_j, U_{j+1}) := a v(x_j + \Delta x/2) - \kappa v'(x_j + \Delta x/2)$.

b) Use Δt to denote the time step. Show that the numerical scheme

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x}[F(U_j^n, U_{j+1}^n) - F(U_{j-1}^n, U_j^n)]$$

is consistent with the convection-diffusion equation.

c) Write down the stability condition of this numerical scheme.

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Part II: Optimization

1. [10 marks] Let $f : S \to R$, where $S \subseteq R^n$ is a nonempty convex set. Let $f_S : S \to R$ denote the convex function such that $f_S(x) \leq f(x)$ for all $x \in S$; and if g is any other convex function for which $g(x) \leq f(x)$ for all $x \in S$, $f_S(x) \geq g(x)$ for all $x \in S$. Assume that the minima of f over S exist. Show that $\min\{f(x) : x \in S\} = \min\{f_S(x) : x \in S\}$, and that $X^* \subseteq X_S^*$, where

$$X^* = \{x^* \in S : f(x^*) \leq f(x), \forall x \in S\},$$
$$X_S^* = \{x^* \in S : f_S(x^*) \leq f_S(x), \forall x \in S\}.$$

2. [15 marks] Consider the problem

$$\begin{aligned} \min \quad & f(x) \\ s.t. \quad & Ax \leq b. \end{aligned}$$

Suppose that $\bar{x}$ is a feasible solution such that $A_1\bar{x} = b_1$ and $A_2\bar{x} < b_2$, where $A^T = (A_1^T, A_2^T)$ and $b^T = (b_1^T, b_2^T)$. Assuming the A_1 has full rank, the matrix P that projects any vector onto the nullspace of A_1 is given by

$$P = I - A_1^T(A_1A_1^T)^{-1}A_1.$$

Let $\bar{d} = -P\nabla f(\bar{x})$.

(a) Show that if $\bar{d} \neq 0$, it is is an improving feasible direction; that is, $\bar{x} + \lambda\bar{d}$ is feasible and $f(\bar{x} + \lambda\bar{d}) < f(\bar{x})$ for $\lambda > 0$ and sufficiently small.

(b) Suppose that $\bar{d} = 0$ and that $u = -(A_1A_1^T)^{-1}A_1\nabla f(\bar{x}) \geq 0$. Show that $\bar{x}$ is a KKT point.

(c) Show that $\bar{d}$ is of the form $\lambda\hat{d}$ for some $\lambda > 0$, where $\hat{d}$ is an optimal solution to the following problem:

$$\begin{aligned} \min \quad & \nabla f(\bar{x})^T d \\ s.t. \quad & A_1 d = 0 \\ & \|d\|^2 \leq 1. \end{aligned}$$

3. [10 marks] Consider the problem

$$\begin{aligned} \min \quad & f(x) \\ s.t. \quad & g_i(x) \leq 0, \quad i = 1, \ldots, m, \end{aligned} \tag{1}$$

where the functions $f : R^n \to R$ and $g_i : R^n \to R$ are differentiable and convex. Let $h_1, \ldots, h_m : R \to R$ be differentiable nondecreasing convex functions.

(i) Show that

$$\phi(x) = f(x) + \sum_{i=1}^{m} h_i(g_i(x))$$

is convex.

(ii) Suppose $\bar{x}$ minimizes ϕ. Let $\bar{\lambda}_i = h_i'(g_i(\bar{x}))$. Show that $\bar{\lambda} = (\bar{\lambda}_1, \ldots, \bar{\lambda}_m)$ is a feasible solution to the Lagrangian dual of the problem (1).

(iii) Find, from $\bar{\lambda}$, a lower bound on the optimal value of the problem (1), and justify your answer.

—— **End of Paper** ——