NATIONAL UNIVERSITY OF SINGAPORE, DEPARTMENT OF MATHEMATICS

Ph.D. Qualifying Examination
Year 2023-2024 Semester I
Computational Mathematics

Time allowed : 3 hours

Instructions to Candidates

1. Use $A4$ size paper and pen (blue or black ink) to write your answers.
2. Write down your student number clearly on the top left of every page of the answers.
3. Write on one side of the paper only. Start each question on a NEW page. Write the question number and page number on the top right corner of each page (e.g. Q1P1, Q1P2, $\cdots$, Q2P1, $\cdots$).
4. This examination paper comprises two parts: Part I contains FOUR (4) questions and Part II contains THREE (3) questions. Answer ALL questions.
5. The total mark for this paper is ONE HUNDRED (100).
6. This is a CLOSED BOOK examination: you are allowed to bring a help sheet.
7. You may use any calculator. However, you should lay out systematically the various steps in the calculations.

Part I: Scientific Computing

1. [15 marks]
Consider the linear system $Ax = b$, where A is the following 3×3 matrix:

$$A = \begin{pmatrix} 3 & -2 & 0 \\ -1 & 3 & -2 \\ 0 & -1 & 3 \end{pmatrix}$$

Find the optimal relaxation factor to achieve fastest convergence rate in the SOR (successive over-relaxation) method.

2. [20 marks]
Consider the ODE system

$$\begin{aligned} u'(t) &= \mathrm{i}Hu(t), \\ u(0) &= u_0, \end{aligned}$$

where $H \in \mathbb{R}^{n\times n}$ is a symmetric matrix and $u : \mathbb{R}_+ \to \mathbb{R}^n$.

   (a) Write down the forward Euler method for the ODE system. Use u_n to denote the solution at the nth time step and Δt to denote the time step.

   (b) Show that there exists a constant C depending only on H such that the numerical solution satisfies

$$\|u(n\Delta t) - u_n\| \le CT\Delta t \cdot \mathrm{e}^{CT\Delta t}\|u_0\|.$$

   (c) Find a numerical scheme such that $\|u_n\| = \|u_0\|$ for all $n > 0$, where u_n denotes the numerical solution at the nth time step.

3. [15 marks]
Consider the partial differential equation

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{1}{\omega(x)}\frac{\partial}{\partial x}\left[\omega(x)\frac{\partial u}{\partial x}\right] \\ u(x,0) &= u_0(x) > 0 \end{aligned}$$

with periodic boundary conditions $u(x+1) = u(x)$.

   (a) Given a positive integer N, let $U_j(t), j = 0, 1, \cdots, N-1$ be the approximation of $u(j/N, t)$. Consider the following finite difference method:

$$\begin{aligned} \frac{\mathrm{d}U_j}{\mathrm{d}t} &= \frac{1}{\omega_j}\frac{\omega_{j+1/2}(U_{j+1} - U_j) - \omega_{j-1/2}(U_j - U_{j-1})}{\Delta x^2}, \\ U_j(0) &= u_0(j/N), \end{aligned}$$

where

$$\omega_j = \omega(j/N), \quad \Delta x = 1/N, \quad U_{-1} = U_{N-1}, \quad U_N = U_0.$$

Show that this semidiscrete scheme satisfies

$$U_j(t) > 0, \qquad j = 0, 1, \cdots, N-1$$

for all $t > 0$.

(b) Show that the above semidiscrete scheme satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{j=0}^{N-1} \omega_j U_j(t) \log U_j(t)\right) \le 0.$$

(c) Find a fully discrete scheme such that

$$U_j^n > 0, \qquad \forall j = 0, 1, \cdots, N-1, \quad \forall n \ge 0,$$
$$\sum_{j=0}^{N-1} \omega_j U_j^{n+1} \log U_j^{n+1} \le \sum_{j=0}^{N-1} \omega_j U_j^n \log U_j^n, \quad \forall n \ge 0,$$

where U_j^n is the approximation of $U_j(t_n)$ with t_n being the nth time step.

4. [15 marks]
Consider the linear advection equation

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0,$$
$$u(x, 0) = u_0(x).$$

Below we assume that a uniform spatial grid is used to discretize the equation, and we use the U_j^n to denote the approximation of $u(x_j, t_n)$, with x_j being the jth grid point and t_n being the nth time step. Apply von Neumann stability analysis to the numerical scheme

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x}(U_{j+1/2}^n - U_{j-1/2}^n),$$

where

$$U_{j+1/2}^n = U_j^n + \frac{U_{j+1}^n - U_{j-1}^n}{4}.$$

Show that the scheme is unconditionally unstable.
[Hint: Focus on the modes with small frequencies.]

Part II: Optimization

1. [12 marks]

   Let $f : R^n \to R$ is convex. Prove the statements below:

   (i) For any bounded set $S \subset R^n$, f is bounded from below and above on S.

   (ii) For any bounded set $S \subset R^n$, there exists a constant c such that $|f(x) - f(y)| \leq c\|x - y\|$ for all $x, y \in S$.

2. [8 marks]

   Let $f_j : R \to R$, $j = 1, \ldots, n$, be differentiable. Consider the problem:

$$\begin{aligned} \min \quad & \sum_{j=1}^{n} f_j(x_j) \\ s.t. \quad & \sum_{j=1}^{n} x_j = 1 \\ & x_j \geq 0 \quad \text{for } j = 1, \ldots, n. \end{aligned}$$

   Suppose that $\bar{x} = (\bar{x}_1, \ldots, \bar{x}_n)^T \geq 0$ solves the problem. Letting $\delta_j = df_j(\bar{x}_j)/dx_j$, show that there exists a scalar κ such that

$$\delta_j \geq \kappa \quad \text{and} \quad (\delta_j - \kappa)\bar{x}_j = 0 \quad \text{for } j = 1, \ldots, n.$$

3. [15 marks]

   Consider the following problem

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

   where $f : R^n \to R$ is *concave*, A is a $m \times n$-matrix and $X = \text{conv}(x_1, \ldots, x_p)$ is the convex hull with $x_1, \ldots, x_p \in R^n$ as its vertices. Let $\theta(u) = \inf\{f(x) + u^T(Ax - b) : x \in X\}$ for $u \in R^m$ be the Lagrangian dual function.

   (i) Show that $\theta : R^m \to R$ is concave.

   (ii) For each vertex x_i of X, let U_i be the set of $u \in R^m$ such that

$$x_i \in \text{argmin}\{f(x) + u^T(Ax - b) : x \in X\}.$$

   Express $\theta(u)$ for $u \in U_i$ explicitly in terms of x_i and show that the restriction of θ to U_i, $\theta|_{U_i}$, is an affine function, that is, in the form of $\alpha + h^T u$ for some $\alpha \in R$ and $h \in R^m$.

   (iii) Show $\cup_{i=1}^{p} U_i = R^m$, that is, for any $u \in R^m$ there exists U_i containing u.

   (iv) For each $u \in R^m$, express the subdifferential $\partial\theta(u)$ explicitly in terms of $x_1, \ldots, x_p$, and justify your answer.