

NATIONAL UNIVERSITY OF SINGAPORE, DEPARTMENT OF MATHEMATICS

**Ph.D. Qualifying Examination
Year 2024-2025 Semester II
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, ..., Q2P1, ...).
 4. This examination paper comprises two parts: Part I contains THREE (3) 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
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Part I: Scientific Computing

Question 1 [25 marks]

Let A be non-singular. Show that

$$\min\left\{\frac{\|\delta A\|_2}{\|A\|_2} : A + \delta A \text{ is singular}\right\} = \frac{1}{k_2(A)},$$

where $k_2(A)$ denotes the 2-norm condition number of A .

Question 2 [20 marks]

Let's solve the problem

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0, \quad 0 \leq x \leq 1, \quad 0 \leq t \leq T,$$

with

$$\begin{cases} u(0, t) = u_1(t), \\ u(1, t) = u_2(t), \end{cases} \quad 0 \leq t \leq T,$$

and

$$u(x, 0) = \phi(x), \quad 0 \leq x \leq 1,$$

using Crank-Nicolson Implicit Scheme. Prove the convergence of the Crank-Nicolson Implicit Scheme.

Question 3 [20 marks]

Show that the initial value problem

$$\frac{dy}{dx} = -\sqrt{|1 - y^2|}, \quad y(0) = 1,$$

is not well-posed.

Part II: Optimization

Question 1 [8 marks]

Prove the following convexity results.

1. Assume $S \subseteq \mathbf{R}^n$ is a nonempty convex set. Show

$$C := \{(x, \lambda) \in \mathbf{R}^{n+1} : x/\lambda \in S, \lambda > 0\} \cup \{(0, 0)\}$$

is a convex cone.

2. Assume $f : \mathbf{R}^n \rightarrow \mathbf{R} \cup \{+\infty\}$ is a proper convex function. Define the *perspective function* of f as

$$f^\pi(x, \lambda) := \begin{cases} \lambda f\left(\frac{x}{\lambda}\right) & \text{if } \lambda > 0 \\ 0 & \text{if } x = 0 \text{ \& } \lambda = 0 \\ +\infty & \text{otherwise.} \end{cases}$$

Show that $f^\pi : \mathbf{R}^{n+1} \rightarrow \mathbf{R} \cup \{+\infty\}$ is a convex function.

Question 2 [12 marks]

Assume $f : \mathbf{R}^n \rightarrow \mathbf{R}$ is a continuously twice differentiable convex function. Consider the following optimization problem

$$\begin{aligned} \min_x & f(x) \\ \text{s.t. } & x \geq 0, \end{aligned} \tag{1}$$

which can be transformed into the following unconstrained program

$$\min_{y \in \mathbf{R}^n} g(y), \tag{2}$$

where $g(y_1, y_2, \dots, y_n) = f(y_1^2, y_2^2, \dots, y_n^2)$. Assume \bar{y} is a first-order stationary solution to (2).

1. Give a counterexample of f to show that \bar{y} may not be an optimal solution to (2).
2. Write down the KKT conditions for the optimization problem (1).
3. Assume in addition that \bar{y} is a second-order stationary solution to (2). Prove that $\bar{x} = (\bar{y}_1^2, \bar{y}_2^2, \dots, \bar{y}_n^2)$ is the optimal solution to (1).

Question 3 [15 marks]

Assume $f : \mathbf{R}^n \rightarrow \mathbf{R}$ is a differentiable convex function with partial derivatives satisfying the following componentwise Lipschitz condition

$$\left| \frac{\partial f(x + \eta e^j)}{\partial x_j} - \frac{\partial f(x)}{\partial x_j} \right| \leq L|\eta| \quad \forall j = 1, \dots, n, \eta \in \mathbf{R}, x \in \mathbf{R}^n,$$

where $L > 0$ is the Lipschitz constant and e^j is the j -th coordinate unit vector. To solve $\min_{x \in \mathbf{R}^n} f(x)$, consider the *steepest coordinate descent method* with a given initial point x^0 :

Algorithm 1

Step 0. Set $k = 0$.

Step 1. Let j_k be the index $j = 1, \dots, n$ that maximizes $\left| \frac{\partial f(x^k)}{\partial x_j} \right|$.

Step 2. Set

$$x^{k+1} = x^k - \frac{1}{L} \frac{\partial f(x^k)}{\partial x_{j_k}} e^{j_k}.$$

Step 3. Replace k by $k + 1$ and go to **Step 1**.

Define the level set $S := \{x : f(x) \leq f(x^0)\}$ and the diameter of S as $D := \max_{x, y \in S} \|x - y\|_2$. Assume $D < \infty$ and $x^* \in \arg \min_{x \in \mathbf{R}^n} f(x)$.

1. Show

$$f(x^{k+1}) - f(x^k) \leq -\frac{1}{2nL} \|\nabla f(x^k)\|_2^2.$$

2. Show

$$\frac{f(x^{k+1}) - f(x^k)}{[f(x^k) - f(x^*)]^2} \leq -\frac{1}{2nL\|x^k - x^*\|^2}.$$

3. Show

$$f(x^k) - f(x^*) \leq \frac{2nLD^2}{k}.$$