NATIONAL UNIVERSITY OF SINGAPORE, DEPARTMENT OF MATHEMATICS

Ph.D. Qualifying Examination
Year 2025-2026 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 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]

Given $A \in \mathbf{R}^{10\times 10}$ with $\|A\|_2 = 1$. Compute

$$\left\| \begin{bmatrix} I & A \\ 0 & I \end{bmatrix} \right\|_2.$$

Question 2 [20 marks]

Find out $\psi(h, t_n)$ such that the order of the following numerical method

$$y_0 = 0.5, \quad y_{n+1} = \psi(h, t_n) + [y_n - (t_n+1)^2](1 + h + \frac{h^2}{2!} + \cdots + \frac{h^k}{k!})$$

applied to the initial value problem

$$\begin{aligned} y' &= y - t^2 + 1, \quad t \geq 0, \\ y(0) &= 0.5, \end{aligned}$$

is k.

Question 3 [20 marks]

Apply the third-order Taylor series method

$$\begin{aligned} y_{n+1} &= y_n + hf(x_n, y_n) + \frac{h^2}{2} f'(x_n, y_n) + \frac{h^3}{6} f''(x_n, y_n), \ n = 0, 1, 2, \cdots, \\ y_0 &= -1, \end{aligned}$$

and the third-order Runge-Kutta method

$$\begin{aligned} \hat{y}_{n+1} &= \hat{y}_n + \frac{1}{9}(2K_1 + 3K_2 + 4K_3), \ n = 0, 1, 2, \cdots, \\ \hat{y}_0 &= -1, \end{aligned}$$

where

$$\begin{aligned} K_1 &= hf(x_n, \hat{y}_n), \\ K_2 &= hf(x_n + \frac{1}{2}h, \hat{y}_n + \frac{1}{2}K_1), \\ K_3 &= hf(x_n + \frac{3}{4}h, \hat{y}_n + \frac{3}{4}K_2), \end{aligned}$$

to the initial value problem

$$y' = y + x, \quad y(0) = -1.$$

Compute

$$(y_1 + y_2) - (\hat{y}_1 + \hat{y}_2)$$

with $h = 0.001$ and $h = 0.002$, respectively.

Part II: Optimization

Question 1 [8 marks]

Let $S = \{(-1, 0), (1, 0), (0, 1)\}$ and denote by $\text{conv}(S)$ the convex hull of S.

1. Rewrite $x = (0, 0, 1/2)$ as a convex combination of th points in S.
2. Note that since $\text{conv}(S)$ is polyhedral, it can be expressed as $\text{conv}(S) = \{x : Ax \leq b\}$ for a certain matrix A and vector b. Figure out A and b.

Question 2 [15 marks]

Let $f : \mathbf{R}^n \to \mathbf{R}$ be a differentiable function with L-Lipschitz continuous gradient, that is,

$$\|\nabla f(x) - \nabla f(y)\|_2 \leq L\|x - y\|_2 \text{ for all } x, y \in \mathbf{R}^n.$$

Assume that the infimum $f^* := \inf_x f(x) > -\infty$. Consider the inexact gradient descent method:

$$x^{k+1} = x^k - \alpha(\nabla f(x^k) + e^k),$$

where $e^k \in \mathbf{R}^n$ is an error term (e.g., due to approximation, or numerical precision), and $\alpha \in (0, 1/L]$ is a fixed step size. Answering the following questions:

1. Prove that
$$f(x^{k+1}) \leq f(x^k) - \frac{\alpha}{2}\|\nabla f(x^k)\|_2^2 + \frac{\alpha}{2}\|e^k\|_2^2$$
2. Suppose the error sequence satisfies $\sum_{k=1}^{\infty} \|e^k\|_2^2 < \infty$. Prove that if the iterates $\{x^k\}_k$ has an accumulated point $\bar{x}$, then it must satisfy $\nabla f(\bar{x}) = 0$.
3. Assume additionally that f is strongly convex. Show that
$$\lim_{k\to\infty} f(x^k) = f^*.$$

Question 3 [12 marks]

A Support Vector Machine (SVM) is a supervised learning model for binary classification. More specifically, an SVM seeks a hyperplane

$$H = \{x \in \mathbf{R}^n : w^\top x + b = 0\}$$

that classifies a point x according to $\text{sign}(w^\top x + b)$, where

$$\text{sign}(t) = \begin{cases} 1 & \text{if } t \geq 0 \\ -1 & \text{if } t < 0. \end{cases}$$

Given training data $\{(x^i, y_i)\}_{i=1}^m$ with $x^i \in \mathbf{R}^n$ and labels $y_i \in \{-1, 1\}$, the learning problem of finding (w, b) can be formulated as the following nonsmooth convex optimization problem

$$\min_{w,x} \sum_{i=1}^{m} \max\{0, 1 - y_i(w^\top x^i + b)\} + \lambda\|w\|_2^2, \tag{1}$$

where λ is a fixed positive constant. Answer the following questions.

1. Show that the optimal solution of (1) can also be obtained by solving the constrained quadratic optimization problem:

$$\begin{aligned} \min_{w,\xi,b} \; & \sum_{i=1}^{m} x_i + \lambda \|w\|_2^2 \\ \text{s.t. } & 1 - y_i(w^\top x^i + b) \le \xi_i, \;\; \forall i = 1, \dots, m \\ & \xi_i \ge 0 \; \forall i = 1, \dots, m. \end{aligned} \tag{2}$$

2. Write down the Karush-Kuhn-Tucker (KKT) conditions for (2).

3. Derive the dual problem of (2).

4. Suppose $\{x^i\}_{i=1}^m$ are not directly available, but we have access to the Kernel matrix K where the (i, j)-th entry of K is given by the inner product $K_{ij} = \langle x^i, x^j \rangle$. We aim to do prediction for a new data point x^0 where all the inner products $\langle x^i, x^0 \rangle \; \forall i = 1, \dots, m$ are assumed to be known. Explain how this process can be done using the dual representation.