NATIONAL UNIVERSITY OF SINGAPORE, DEPARTMENT OF MATHEMATICS

Ph.D. Qualifying Examination
Year 2022-2023 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, $\cdots$, 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]

   Suppose $A = (a_{ij}) \in \mathbf{R}^{n\times n}$ is symmetric positive definite. Prove that the Gauss-Seidel method for linear system $Ax = b$ converges.

2. [15 marks]

   CG method for $Ax = b$ with A symmetric can be stated as follows.

   Algorithm 1 *(The CG method)*
   Given $x_0 \in \mathbf{R}^n$, $d_0 = -(Ax_0 - b) = -r_0$.
   For $k = 0, 1, 2, \cdots,$

   $\alpha_k = -\frac{(Ax_k - b)^T d_k}{d_k^T A d_k} = -\frac{r_k^T d_k}{d_k^T A d_k}$;
   $x_{k+1} = x_k + \alpha_k d_k$;
   $r_{k+1} = Ax_{k+1} - b$;
   $\beta_k = \frac{r_{k+1}^T A d_k}{d_k^T A d_k}$;
   $d_{k+1} = -r_{k+1} + \beta_k d_k$.

   Denote the linear space spanned by vectors $y_1, y_2, \cdots, y_m$ by $[y_1, y_2, \cdots, y_m]$, i.e.,

   $$[y_1, y_2, \cdots, y_m] = \{y \in \mathbf{R}^n,\ y = \sum_{i=1}^{m} a_i y_i,\ a_i \in \mathbf{R}\}.$$

   Prove that for $m = 0, 1, \cdots,$

   $$[d_0, d_1, \cdots, d_m] = [r_0, r_1, \cdots, r_m] = \left[r_0, Ar_0, \cdots, A^m r_0\right].$$

3. [20 marks]

   Derive the most accurate linear 2-step method for the initial-value problem

   $$y' = f(x, y), \quad a \le x \le b, \qquad y(a) = \alpha.$$

4. [15 marks]

   Show that the Midpoint method, the Modified Euler's method and Heun's method give the same approximations to the initial value problem

   $$y' = -y + t + 1, \quad 0 \le t \le 1, \qquad y(0) = 1,$$

   for any choice of h.

Part II: Optimization

1. [8 marks]

(i) Let S be a nonempty convex set in R^n, and let $f : R^n \to R$ be defined as follows:

$$f(x) = \inf\{\|y - x\| : y \in S\}.$$

Show that f is convex.

(ii) If the convexity of S is not assumed, is the function f defined in (i) still convex? Prove it if your answer is YES, or disprove it by giving a counterexample if your answer is NO.

2. [15 marks]

Consider the program

$$\begin{array}{ll} \min & f(x) \\ s.t. & g_i(x) \le 0, \quad i = 1, 2, \ldots, m, \end{array} \tag{1}$$

where $f : R^n \to R$ and $g_i : R^n \to R$, $i = 1, \ldots, m$, are differentiable functions.

(i) Suppose that at $\bar{x} \in R^n$ there exists $d \in R^n$ satisfying

$$\nabla f(\bar{x})^T d > 0, \quad \nabla g_i(\bar{x})^T d > 0 \quad i = 1, 2, \ldots, m.$$

Can $\bar{x}$ be an optimal solution to the program (1)? Justify your answer.

(ii) Suppose that at $\bar{x} \in R^n$ there is no $d \in R^n$ satisfying

$$\nabla f(\bar{x})^T d > 0, \quad \nabla g_i(\bar{x})^T d \ge 0 \quad i = 1, 2, \ldots, m.$$

(a) Show that there exists $\lambda = (\lambda_1, \ldots, \lambda_m) \ge 0$ satisfying

$$\nabla f(\bar{x}) + \sum_{i=1}^{m} \lambda_i \nabla g_i(\bar{x}) = 0. \tag{2}$$

(b) Is $\bar{x}$ a KKT-point to the program (1)? Justify your answer.

(iii) Supppose that $f : R^n \to R$ and $g_i : R^n \to R$, $i = 1, \ldots, m$, are convex. Show that $\bar{x}$ is a minimizer of the function $f(x) + \sum_{i=1}^m \lambda_i g_i(x)$ for $x \in R^n$, where λ satisfies (2).

(iv) Supppose that $f : R^n \to R$ and $g_i : R^n \to R$, $i = 1, \ldots, m$, are convex. Find a lower bound of the optimal objective value of the program (1) in terms of λ and $\bar{x}$, by using the duality.

3. [12 marks]

Let $\theta(u) = \inf\{f(x) + u^T g(x) : x \in X\}$ be the dual function of the problem $\min f(x)$ subject to $g(x) \le 0$ and $x \in X$. Assume that X is compact, $f : R^n \to R$ and $g : R^n \to R^m$ are continuous.

(i) Show that the directional derivative $\theta'(u;d)$ of θ at u in the direction d is a continuous function of d.

In the subquestions (ii) and (iii), suppose that the shortest subgradient $\bar{\xi}$ of θ at $\bar{u}$ is not equal to zero.

(ii) Show that $d = \bar{\xi}$ is an ascent direction of θ at $\bar{u}$.

(iii) Show that there exists an $\delta > 0$ such that $\|\xi - \bar{\xi}\| < \delta$ implies that $d = \xi$ is an ascent direction of θ at $\bar{u}$.