NATIONAL UNIVERSITY OF SINGAPORE, DEPARTMENT OF MATHEMATICS

Ph.D. Qualifying Examination
Year 2021-2022 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 an OPEN BOOK examination: you are allowed to use any book or lecture notes (hard copies or PDF), but you are not allowed to search online or discuss with others.
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]

   (a) Given $A \in \mathbf{R}^{3\times 3}$ with

   $$\|A\|_F = \sqrt{14}, \quad \|A\|_2 = 3, \quad \det(A) = -6.$$

   Find all singular values of A.

   (b) Given $A \in \mathbf{R}^{10\times 10}$. Assume

   $$\text{rank}(A) = 6, \qquad \min_{\substack{B \in \mathbf{R}^{10\times 10} \\ \text{rank}(B) \le 5}} \|A - B\|_2 = 3.$$

   Find the smallest non-zero singular value of A.

2. [15 marks]

   Consider the initial value problem

   $$\begin{aligned} y' &= y + x, \qquad 1 \le x \le 2, \\ y(1) &= 1. \end{aligned}$$

   Apply the third-order Taylor Series Method and the third-order Runge-Kutta method:

   $$y_{n+1} = y_n + \frac{1}{9}(2K_1 + 3K_2 + 4K_3),$$

   where

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

   to approximate $y(2)$ with the step size h. The approximated values are denoted as $y_T(2,h)$ and $y_R(2,h)$, respectively. Compute

   $$y_T(2,h) - y_R(2,h)$$

   with $h = 0.1$, $h = 0.01$ and $h = 0.001$, respectively.

3. [15 marks]

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

   $$y' = (xy)^3 - (\frac{y}{x})^2, \quad a \le x \le b, \qquad y(a) = \alpha.$$

4. [20 marks]

The equation

$$u_t - u_{xx} = 0 \tag{1}$$

is approximated at the point (ih, jk) by the difference equation

$$\theta(\frac{u_{i,j+1} - u_{i,j-1}}{2\tau}) + (1-\theta)(\frac{u_{i,j} - u_{i,j-1}}{\tau}) - \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} = 0.$$

Find the value of θ such that the local truncation error at this point is of the form

$$\frac{\tau^2}{6}(\frac{\partial^6 U}{\partial x^6})_{i,j} + \mathbf{O}(\tau^{\mathbf{3}} + \mathbf{h^4}),$$

where U is the exact solution of the pde (1).

Part II: Optimization

1. [10 marks] Let A be an $m \times n$-matrix. Consider the following two systems:

   S1: $Ax \geq 0$.

   S2: $A^T y = 0$, $y \geq 0$.

   (i) Show that, for each $i \in \{1, \ldots, m\}$, exactly one of the following systems has a solution:

   System I: $Ax \geq 0$ with $A_i x > 0$,

   System II: $A^T y = 0$, $y \geq 0$, with $y_i > 0$,

   where A_i is the i-th row of A.

   (ii) Show that there exist solutions x^* to **S1** and y^* to **S2** such that $Ax^* + y^* > 0$.

2. [10 marks] Let $f_1, \ldots, f_m$ be convex functions on R^n. Let

$$f(x) = \inf\{f_1(x_1) + \cdots + f_m(x_m) : x_i \in R^n, x_1 + \cdots + x_m = x\}$$

   and $F = \mathrm{epi} f_1 + \cdots + \mathrm{epi} f_m$.

   (i) Show that $f(x) = \inf\{\mu : (x, \mu) \in F\}$.

   (ii) Show that f is a convex function on R^n.

3. [15 marks] Let $A \in R^{n \times n}$ be symmetric positive definite, $b \in R^n$ and $\phi(x) := \frac{1}{2} x^T A x - b^T x$. Let $d_0, d_1, \ldots, d_{n-1}$ be a set of linearly independent vectors in R^n. Define a set of vectors $p_0, p_1, \ldots, p_{n-1}$ in R^n by

$$p_0 = d_0, \quad p_k = d_k - \sum_{i=0}^{k-1} \frac{d_k^T A p_i}{p_i^T A p_i} p_i \text{ for } k \geq 1.$$

   (i) Show that the vectors $p_0, p_1, \ldots, p_{n-1}$ are A-conjugate.

   (ii) Let $x_k \in R^n$ be the minimizer of ϕ over the set $a + \mathrm{span}\{d_0, d_1, \ldots, d_{k-1}\}$ for some $a \in R^n$. Show that $x_{k+1} = x_k + \alpha_k p_k$, where $\alpha_k = -p_k^T \nabla\phi(x_k)/(p_k^T A p_k)$, is a minimizer of ϕ over the set $a + \mathrm{span}\{d_0, d_1, \ldots, d_k\}$.