NATIONAL UNIVERSITY OF SINGAPORE, DEPARTMENT OF MATHEMATICS

Ph.D. Qualifying Examination
Year 2023-2024 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. [17 marks]

   Consider the matrix

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

   Find an upper triangular matrix U and a unit lower triangular matrix L such that $A = UL$.

2. [16 marks]

   Consider the ODE system

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

   and the following numerical scheme:

$$\begin{aligned} u^{(1)} &= u_n + \frac{h}{3} f(u_n), \\ u^{(2)} &= u^{(1)} + \frac{h}{2} f(u^{(1)}), \\ u_{n+1} &= u^{(2)} + h f(u^{(2)}), \end{aligned}$$

   where h is the time step, u_n approximates $u(nh)$, and $u^{(1)}$ and $u^{(2)}$ are intermediate variables.

   i. Write down Butcher's tableau of the numerical scheme and determine its numerical order.

   ii. Apply the numerical scheme to the equation

$$\begin{aligned} u'(t) &= \mathrm{i}\lambda u(t), \qquad \lambda \in \mathbf{R}, \\ u(0) &= 1. \end{aligned} \tag{1}$$

   Show that the numerical error satisfies

$$|u((n+1)h) - u_{n+1}| \le \frac{(|\lambda|h)^4}{24} + \exp(|\lambda|h)|u(nh) - u_n|.$$

   iii. Derive an estimation of the error $|u(nh) - u_n|$ for (1).

3. [16 marks]

   Consider the linear advection equation

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} &= 0, \\ u(x,0) = u_0(x) &> 0 \end{aligned}$$

with the periodic boundary condition $u(x+1,t) = u(x,t)$, $\forall t > 0$. 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:

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

where

$$F(U^{(1)}, U^{(2)}) = \begin{cases} \dfrac{U^{(1)} - U^{(2)}}{\log U^{(1)} - \log U^{(2)}}, & \text{if } U^{(1)} \neq U^{(2)}, \\ U^{(1)}, & \text{if } U^{(1)} = U^{(2)}, \end{cases}$$

$$\Delta x = 1/N, \quad U_{-1} = U_{N-1}, \quad U_N = U_0.$$

i. Show that $[F(u(x_j,t), u(x_{j+1},t)) - F(u(x_{j-1},t), u(x_j,t))]/\Delta x$ is a first-order approximation of $\partial_x u(x_j, t)$ when the function u is positive.

ii. Show that the numerical scheme satisfies

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

and

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

iii. Find a fully discrete scheme such that

$$\sum_{j=0}^{N-1} U_j^{n+1} \log U_j^{n+1} \leq \sum_{j=0}^{N-1} U_j^n \log U_j^n, \quad \forall n > 0,$$

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

4. [16 marks]

Consider the equation

$$\begin{aligned} -u''(x) &= 2, \quad x \in (0, 2), \\ u'(0) &= u(0), \quad u'(2) = 0. \end{aligned}$$

Discretize the equation on the uniform grid with two cells:

$$x_0 = 0, \quad x_1 = 1, \quad x_2 = 2.$$

Use the finite element method to solve the problem.

Part II: Optimization

1. [8 marks]

   Suppose that $a_0, a_1, \ldots, a_m$ are fixed elements of R^n. Show that the inner product $\langle a_0, y\rangle \leq \max \{\langle a_1, y\rangle, \ldots, \langle a_m, y\rangle\}$ for all $y \in R^n$ if and only if $a_0 \in \text{conv}(a_1, \ldots, a_m)$, where $\text{conv}(a_1, \ldots, a_m)$ denotes the convex hull of $a_1, \ldots, a_m$.

2. [15 marks]

   Let $f : R^n \to R$ be a continuously differentiable convex function and $S \subset R^n$ be a closed convex set. Define the projection map $\Pi_S : R^n \to S$ by

   $$\Pi_S(x) = \text{argmin}\{\|y - x\| : y \in S\}.$$

   Show that the following statements are equivalent.

   (i) x^* is an optimal solution to the problem

   $$\begin{array}{ll} \min & f(x) \\ \text{s. t.} & x \in S. \end{array}$$

   (ii) $x^* \in S$ satisfies

   $$\nabla f(x^*)^T(x - x^*) \geq 0 \qquad \forall\, x \in S.$$

   (iii)

   $$x^* = \Pi_S\big(x^* - \nabla f(x^*)\big).$$

3. [12 marks]

   Consider the following problem:

   $$\begin{array}{ll} \min & f(x) \\ s.t. & g(x) \leq 0 \\ & x \in S, \end{array} \tag{2}$$

   where S is a nonempty convex set in R^n, and $f : R^n \to R$ and $g : R^n \to R^m$ are convex. Consider the perturbation function $\phi : R^n \to R$ defined below:

   $$\phi(y) = \inf\{f(x) : g(x) \leq y,\ x \in S\}.$$

   Assume that there exists an open neighborhood N of the origin such that $\phi(y) \neq \pm\infty\ \forall\, y \in N$.

   (i) Prove that ϕ is convex on N.

   (ii) Suppose that there exists an $\hat{x} \in \text{int}(S)$ such that $g(\hat{x}) < 0$ (Slater's constraint qualification). Find a subgradient of ϕ at $y = 0$ in terms of the optimal solution to the dual of the problem (2). (*Hint: You may consider the dual of* $\inf\{f(x) : g(x) - y \leq 0,\ x \in S\}$.)