S.-T. Yau College Student Mathematics Contests 2018

Applied Math. and Computational Math.

Individual (5 problems)

1. We consider the following convection-diffusion equation

$$(1) \qquad u_t + a u_x = b u_{xx}, \qquad 0 \le x < 1$$

with an initial condition $u(x,0) = f(x)$ and periodic boundary condition, where a and $b > 0$ are constants. The first order IMEX (implicit-explicit) time discretization and second order central spatial discretization are used to give the following scheme:

$$(2) \qquad \frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} = b\frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{\Delta x^2}$$

with a uniform mesh $x_j = j\Delta x$ with spatial mesh size Δx and time step Δt. Here u_j^n is the numerical solution approximating the exact solution of (1) at $x = x_j$ and $t = n\Delta t$. Prove that the scheme is L^2 stable under the very mild time step restriction

$$(3) \qquad \Delta t \le c$$

with a constant c which is independent of Δx. Can you determine the dependency of c on the two constants a and b in (1)?

2. Velocity-Verlet method.

(a) Recast the following Newtonian formula for the acceleration and potential force

$$q''(t) = -\nabla V(q),$$

into a Hamiltonian system and show that the corresponding map on the phase space is symplectic.

(b) Show that the velocity-Verlet (recovered many times: Delambre 1791, Størmer in 1907, Cowell & Crommelin 1909, Verlet 1960s) method

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{\Delta t}{2}\nabla V(q_n); \\ q_{n+1} &= q_n + \Delta t p_{n+1/2}; \\ p_{n+1} &= p_{n+1/2} - \frac{\Delta t}{2}\nabla V(q_{n+1}) \end{aligned}$$

is symplectic and is second order accurate.

Hint: Let $u(t) = (p(t), q(t))$ be a solution of the Hamiltonian system with initial data $u_0 = (p_0, q_0)$ and we view the solution $u(t)$ as a map map on the phase space $\varphi_t : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d \times \mathbb{R}^d$ $\varphi_t(u_0) = u(t)$. We call the flow map is symplectic *if its Jacobian*

$$\Phi_t(u_0) = \frac{\partial \varphi_t(u_0)}{\partial u_0} = \begin{pmatrix} \frac{\partial p(t)}{\partial p_0} & \frac{\partial p(t)}{\partial q_0} \\ \frac{\partial q(t)}{\partial p_0} & \frac{\partial q(t)}{\partial q_0} \end{pmatrix}$$

satisfies $\Phi_t(u_0)^{\mathrm{T}} J \Phi_t(u_0) = J$ for any $u_0 \in \mathbb{R}^d \times \mathbb{R}^d$. Here $J = \left(\begin{smallmatrix} 0 & I \\ -I & 0 \end{smallmatrix}\right)$.

A scheme $\varphi_n(u_0), n = 1, 2 \ldots,$ is symplectic if the map $\varphi_n(u_0)$ is symplectic.

3. We begin with some definitions.

(1) A graph G is a pair $G = (V, E)$ where V is a finite set, called the vertices of G, and E is a subset of $P_2(V)$ (*i.e.*, a set E of (unordered) two-element subsets of V), called the edges of G. A simple graph G is a graph without loops (edge that connects a vertex to itself) or multiple edges between any pair of vertices. The order of the graph is $|V|$. We often put $V = \{v_1, v_2, \cdots, v_n\}$ and $E = \{v_i v_j |\ v_i \text{ and } v_j \text{ are adjacent}\}$.

(2) Two vertices x and y are adjacent if $xy \in E$. The neighborhood of a vertex x, denoted by $N_G(x)$ or $N(x)$, is the set of vertices that is adjacent to x. The degree of a vertex x, denoted by $d_G(x)$ or $d(x)$, is $|N(x)|$ (*i.e.* the number of vertices that is adjacent to x).

(3) A path is a collection of distinct vertices $v_{i_1} v_{i_2} \cdots v_{i_k}$ such that $v_{i_j} v_{i_{j+1}} \in E$ for all j, $1 \leq j < k$. v_{i_1} and v_{i_k} are the ends of the path. A Hamiltonian path P is a path containing all vertices of the graph. A cycle is a closed path with $v_{i_1} = v_{i_k}$. A Hamiltonian cycle is a cycle containing all vertices of the graph. A graph is called Hamiltonian if it has a Hamiltonian cycle.

(4) A graph G is (Hamilton) connected, if for every pair of vertices there is a (Hamiltonian) path between them.

An example of a simple graph: $V = \{v_1, v_2, v_3, v_4\}$ and $E = \{v_1v_2, v_2v_3,\ v_3v_4, v_2v_4\}$. In this graph, the order of the graph is 4, $N(v_1) = \{v_2\}$, $N(v_4) = \{v_2, v_3\}$, $d(v_3) = 2$, $d(v_2) = 3$ and $v_1v_2v_4v_3$ is a Hamiltonian path with ends v_1 and v_3.

Let G be a simple graph of order n. Suppose that the degree sum of any pair of nonadjacent vertices is at least $n+1$. Show that G is Hamilton-connected (*i.e.* between any pair of vertices x and y, there is a Hamiltonian path in which x and y are the ends).

4. Define the Hermite polynomials as

$$H_n(x) = (-1)^n \exp(\frac{x^2}{2}) \frac{d^n}{dx^n}[\exp(-\frac{x^2}{2})], \quad x \in (-\infty, +\infty),\ n = 0, 1, 2, \cdots. \tag{4}$$

(a) Prove the weighted orthogonality of the Hermite polynomials:

$$\langle H_n(x), H_m(x)\rangle_\rho \triangleq \int_{-\infty}^{+\infty} \rho(x) H_n(x) H_m(x) dx = n!\sqrt{2\pi}\delta_{n,m}, \tag{5}$$

where $\rho(x) = \exp(-\frac{x^2}{2})$.

(b) Prove the three recurrence formula:

$$H_{n+1}(x) = xH_n(x) - nH_{n-1}(x), \quad n \geq 1, \tag{6}$$

and then show that for all $n \geq 1$, $H_n(x)$ and $H_{n-1}(x)$ share no common roots.

(c) Use the recurrence formula and induction to prove the differential relation:

$$\frac{d}{dx} H_n(x) = nH_{n-1}(x), \quad n \geq 1, \tag{7}$$

and then prove that H_n is an eigenfunction of the following eigenvalue problem

$$xu'(x) - u''(x) = \lambda u. \tag{8}$$

You need to find the eigenvalue λ_n corresponding to $H_n(x)$.

5. Take $\sigma_i(A)$ to be the i-th singular value of the square matrix $A \in \mathbb{R}^{n\times n}$. Define the *nuclear norm* of A to be

$$\|A\|_* \equiv \sum_{i=1}^{n} \sigma_i(A).$$

(1) Show that $\|A\|_* = \mathrm{tr}(\sqrt{A^T A})$.
(2) Show that $\|A\|_* = \max_{X^T X = I} \mathrm{tr}(AX)$.
(3) Show that $\|A + B\|_* \leq \|A\|_* + \|B\|_*$
(4) Explain informally why minimizing $\|A - A_0\|_{\mathrm{F}}^2 + \|A\|_*$ over A for a fixed $A_0 \in \mathbb{R}^{n\times n}$ might yield a low-rank approximation of A_0.

Notation: The trace of a matrix $\mathrm{tr}(A)$ is the sum $\sum_i a_{ii}$ of its diagonal elements. We define the square root of a symmetric positive semidefinite matrix M to be $\sqrt{M} \equiv UD^{1/2}U^T$, where $D^{1/2}$ is the diagonal matrix containing (nonnegative) square roots of the eigenvalues of M and U contains the eigenvectors of $M = UDU^T$.