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Numerical Analysis II

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Problem 1 **[70 points]**

Consider

$$\begin{cases} \dfrac{\mathrm{d}x}{\mathrm{d}t} = f(t,x), \quad t \in [0,T], \\ x(0) = x_0 \in \mathbb{R}, \end{cases} \tag{1.1}$$

with $f \in C^\infty([0,T] \times \mathbb{R})$ satisfying the Lipschitz condition

$$|f(t,x) - f(t,y)| \le C_f |x-y|, \quad \forall x,y \in \mathbb{R}, \quad \forall t \in [0,T],$$

for some positive constant C_f.

(1a)

(i) **[2 points]** Does (1.1) have a unique solution $x(t) \in C^\infty([0,T])$? Justify.

(ii) **[2 points]** If we regard $x(t)$ also as a function of the initial value x_0, what is the equation satisfied by the derivative with respect to t of $\partial x(t)/\partial x_0$? Is it a linear equation? Justify.

(1b) Consider the Runge-Kutta method

$$x^{k+1} = x^k + \Delta t\big(b_1 f(t_k, x^k) + b_2 f(t_k + c_2\Delta t, x^k + \Delta t f(t_k, x^k))\big), \tag{1.2}$$

where $\Delta t > 0$ is small enough, $T/\Delta t$ is an integer and $t_k = k\Delta t$ for $k \in \mathbb{N}$. Here, b_1, b_2 and c_2 are real parameters.

(i) **[1 points]** The scheme (1.2) is an...

explicit one-step method. ☐	explicit two-step method. ☐
implicit one-step method. ☐	implicit two-step method. ☐

(ii) **[2 points]** Let $\Phi(t_k, x^k, \Delta t)$ be defined by

$$\Phi(t_k, x^k, \Delta t) = b_1 f(t_k, x^k) + b_2 f(t_k + c_2\Delta t, x^k + \Delta t f(t_k, x^k))$$

so that (1.2) can be rewritten in the form

$$x^{k+1} = x^k + \Delta t \Phi(t_k, x^k, \Delta t).$$

Prove, from the definition of consistency, that (1.2) is consistent with (1.1) if and only if $b_1 + b_2 = 1$.

(iii) **[5 points]** Define the truncation error by

$$T_k(\Delta t) = \frac{x(t_{k+1}) - x(t_k)}{\Delta t} - \Phi(t_k, x(t_k), \Delta t).$$

Prove, using Taylor's theorem, that if $b_1 + b_2 = 1$, $c_2 = 1$ and $b_2 c_2 = 1/2$ then (1.2) is of order two as $\Delta t \to 0$.

(iv) **[4 points]** Prove that (1.2) is stable, i.e. there exist positive constants h_0 and C_Φ such that

$$|\Phi(t, x, h) - \Phi(t, y, h)| \le C_\Phi |x - y|,$$

for all $t \in [0, T]$ and for all $x, y \in \mathbb{R}$ and $h \in [0, h_0]$.

(v) **[2 points]** Is (1.2) for solving (1.1) convergent?

(1c) Suppose that (1.2), with $b_1 = b_2 = 1/2$ and $c_2 = 1$, is applied to the initial value problem

$$\begin{cases} \dfrac{\mathrm{d}x}{\mathrm{d}t} = -\lambda x, \quad t \in [0, T], \\ x(0) = 1, \end{cases} \tag{1.3}$$

where λ is a positive real number.

(i) **[4 points]** Show that the sequence $\{x^k\}$ is bounded if and only if $\Delta t \le 2/\lambda$.

(ii) **[5 points]** Use the analytic solution to (1.3), namely $x(t) = \exp(-\lambda t)$, to show further that, for such λ,

$$\left|x(t_k) - x^k\right| \le \frac{1}{6}\lambda^3 T (\Delta t)^2, \qquad \frac{T}{\Delta t} \ge k \ge 0.$$

(1d) Consider the harmonic oscillator system

$$\begin{cases} \dfrac{\mathrm{d}^2 y}{\mathrm{d}t^2} = -y, \quad t \in [0, T], \\ y(0) = y_0 \in \mathbb{R}, \\ y'(0) = y_1 \in \mathbb{R} \end{cases} \tag{1.4}$$

Let $p = y$ and $q = -\mathrm{d}y/\mathrm{d}t$.

(i) **[2 points]** Show that (1.4) can be rewritten in the form

$$\begin{cases} \dfrac{\mathrm{d}p}{\mathrm{d}t} = -q, \\ \dfrac{\mathrm{d}q}{\mathrm{d}t} = p, \\ p(0) = y_0 \in \mathbb{R}, \\ q(0) = -y_1 \in \mathbb{R}, \end{cases}$$

or, equivalently,

$$\begin{cases} \dfrac{\mathrm{d}x}{\mathrm{d}t} = J^{-1}\nabla H(x), \\ x(0) = (y_0, -y_1)^\top = x_0 \in \mathbb{R}^2, \end{cases} \tag{1.5}$$

where $x^\top$ denotes the transpose of x, $x = (p,q)^\top$, $H(x) = H(p,q) = (p^2+q^2)/2$ and $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

(ii) **[2 points]** Let $\Psi(t) = \partial x(t)/\partial x_0$. Prove that Ψ satisfies the equation

$$\begin{cases} \dfrac{\mathrm{d}\Psi}{\mathrm{d}t} = \dfrac{\partial f}{\partial x}\Psi, \\ \Psi(0) = I, \end{cases} \tag{1.6}$$

where I is the 2×2 identity matrix and $f(x) = J^{-1}\nabla H(x)$.

(iii) **[6 points]** Show that trace$(\partial f/\partial x) = 0$ and, using the Jacobi formula

$$\text{trace}\left(\frac{\mathrm{d}\Psi}{\mathrm{d}t}\Psi^{-1}\right) = \frac{1}{\det \Psi}\frac{\mathrm{d}(\det \Psi)}{\mathrm{d}t},$$

prove that

$$\frac{\mathrm{d}(\det \Psi)}{\mathrm{d}t} = 0,$$

or, equivalently, that $\det \Psi$ is preserved where Ψ is the solution to (1.6). Deduce that the flow associated to (1.5) preserves the volume.

(1e) Consider the Improved Euler Scheme given by

$$x^{k+1} = x^k + \frac{1}{2}\Delta t\big[f(x^k) + f(x^k + \Delta t f(x^k))\big], \tag{1.7}$$

where $x^k = \begin{pmatrix} p^k \\ q^k \end{pmatrix}$ and $f(x) = J^{-1}\nabla H(x)$, as above.

(i) **[4 points]** Show that

$$(p^{k+1})^2 + (q^{k+1})^2 = \left(1 + \frac{\Delta t^4}{4}\right)\big((p^k)^2 + (q^k)^2\big).$$

(ii) **[2 points]** Does the scheme (1.7) preserve the Hamiltonian H?

(iii) **[5 points]** Implement the Improved Euler Scheme (1.7) for the harmonic oscillator system (1.4) with initial values $p_0 = 1$ and $q_0 = 0$ and step size $\Delta t = 0.05$. Plot $x(t)$ for $t \in [0, 10]$. Plot the Hamiltonian $H(t)$ for $t \in [0, 10]$. You can use the templates given in `improved_euler.py` and `harmonic_oscillator.py`.

(1f) Consider the scheme

$$\begin{cases} q^{k+1} = q^k + \Delta t p^k, \\ p^{k+1} = p^k - \Delta t q^{k+1}. \end{cases} \tag{1.8}$$

(i) **[4 points]** Is (1.8) symplectic?

(ii) **[2 points]** Write the scheme that is the adjoint to (1.8).

(iii) **[4 points]** Prove that (1.8) does not preserve the Hamiltonian $H(p,q) = \frac{1}{2}(p^2 + q^2)$ but that it does preserve the modified Hamiltonian $\hat{H}(p,q) = \frac{1}{2}(p^2 + q^2) + \frac{\Delta t}{2} pq$.

(iv) **[2 points]** Show that

$$\nabla \hat{H} = \begin{pmatrix} 1 & \frac{\Delta t}{2} \\ \frac{\Delta t}{2} & 1 \end{pmatrix} \nabla H.$$

(1g) **[10 points]** By filling in the template `symplectic_euler.py`, implement (1.8) with initial values $p_0 = 1$ and $q_0 = 0$, step size $\Delta t = 0.05$ and $t \in [0, 10]$. Use the template `symplectic_euler_plot.py` to plot the solutions p and q against time, and plot the trajectory in the (p,q)-plane.

Modify the template `area_preserving.py` to illustrate that the scheme preserves area in the (p,q)-plane by finding the image of the triangle ABC, which has vertices $(p_A^0, q_A^0) = (1, 0)$, $(p_B^0, q_B^0) = (1, 3)$ and $(p_C^0, q_C^0) = (0, 1)$. Compute the solutions using the previous code and plot the triangle both at $t = 0$ and at the end time $t = 10$. Calculate the area of the triangles at time $t = 0$ and $t = 10$ to show area preservation.

HINT: The area of a triangle can be computed using the formula

$$\mathcal{A}_{ABC} = \frac{1}{2}[p_A(q_B - q_C) + p_B(q_C - q_A) + p_C(q_A - q_B)].$$

HINT: To multiply matrices in Python, you can use the `matmul` function from the `numpy` module.

Problem 2 **[30 points]**

Consider

$$\begin{cases} \dfrac{\mathrm{d}x}{\mathrm{d}t} = f(x), \quad t \in [0,T], \\ x(0) = x_0 \in \mathbb{R}^2, \end{cases} \tag{2.1}$$

with $f \in C^\infty(\mathbb{R}^2)$ satisfying the Lipschitz condition

$$\|f(x) - f(y)\| \le C_f \|x - y\|, \quad \forall x, y \in \mathbb{R}^2,$$

for some positive constant C_f.

Consider the numerical scheme

$$x^{k+1} = x^k + \Delta t \int_0^1 f(\theta x^{k+1} + (1-\theta)x^k)\,\mathrm{d}\theta, \tag{2.2}$$

where $\Delta t > 0$ is small enough.

(2a)

(i) **[3 points]** Let $x^k \in \mathbb{R}^2$ and $\Delta t > 0$, and let $G : \mathbb{R}^2 \to \mathbb{R}^2$ be defined by

$$G(y) = x^k + \Delta t \int_0^1 f(\theta y + (1-\theta)x^k)\,\mathrm{d}\theta.$$

Prove that

$$\|G(\xi) - G(y)\| \le \frac{\Delta t\, C_f}{2}\|\xi - y\|, \quad \forall \xi, y \in \mathbb{R}^2,$$

and therefore G is a contraction if $\Delta t\, C_f < 2$.

(ii) **[3 points]** Deduce that (2.2) is well defined, provided that Δt is sufficiently small.

(iii) **[1 points]** The scheme (2.2) is an...

explicit one-step method. ☐	explicit two-step method. ☐
implicit one-step method. ☐	implicit two-step method. ☐

(2b) **[2 points]** By using the change of variables $\zeta = 1 - \theta$, prove that (2.2) is symmetric (*i.e.* it coincides with its adjoint).

(2c) Let $f(x) = J^{-1}\nabla H(x)$ where $H \in C^\infty(\mathbb{R}^2)$ and

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

(i) **[2 points]** Show that

$$\int_0^1 \frac{\mathrm{d}}{\mathrm{d}\theta} H(\theta x^{k+1} + (1-\theta)x^k)\mathrm{d}\theta = \int_0^1 \nabla H(\theta x^{k+1} + (1-\theta)x^k)\mathrm{d}\theta \cdot (x^{k+1} - x^k).$$

(ii) **[5 points]** Deduce that (2.2) is energy preserving in the sense that $H(x^{k+1}) = H(x^k)$.

(2d) Let $H(x) = \frac{1}{2}\|x\|^2$.

(i) **[3 points]** Compute exactly the integral

$$\int_0^1 J^{-1} \nabla H(\theta x^{k+1} + (1-\theta)x^k)\,\mathrm{d}\theta.$$

(ii) **[3 points]** Show that, in this case, the scheme (2.2) can be written explicitly as

$$x^{k+1} = A x^k$$

for some 2×2 matrix A, which you should find.

(iii) **[8 points]** Complete the template `ImpMidPoint.py` to implement the scheme (2.2) for this case. Then use the template `ImpMidPointPlot.py` to plot the solution $x(t) = (p(t), q(t))$ for $t \in [0, 10]$ with initial value $x(0) = (1, 2)^\top$ and step size $\Delta t = 0.1$. On separate axes, plot the Hamiltonian $H(p(t), q(t))$ for $t \in [0, 10]$.

HINT: To multiply matrices in Python, you can use the `matmul` function from the `numpy` module.