

## Final Exam Winter 2021

A total of **80 points** can be obtained in this exam. There are three problems of similar length.

### Problem 1

[28 points]

Let  $\mathbf{A} \in \mathbb{R}^{n \times n}$  be an  $n \times n$  matrix with real entries. We denote by  $\mathbf{A}^\top$  the transpose of  $\mathbf{A}$ . We say that  $\mathbf{A}$  is skew symmetric if  $\mathbf{A}^\top = -\mathbf{A}$ . We also say that a matrix  $\mathbf{B} \in \mathbb{R}^{n \times n}$  is orthogonal if  $\mathbf{B}\mathbf{B}^\top = \mathbf{I}$ , with  $\mathbf{I}$  being the  $n \times n$  identity matrix.

(1a) Let the matrix-valued function  $\mathbf{Y} : \mathbb{R} \rightarrow \mathbb{R}^{n \times n}$  satisfy the linear matrix differential equation

$$\frac{d\mathbf{Y}}{dt} = \mathbf{A}\mathbf{Y}, \quad (1.1)$$

with  $\mathbf{A} \in \mathbb{R}^{n \times n}$  being skew symmetric.

(i) [4 points] Compute  $\frac{d}{dt}(\mathbf{Y}^\top \mathbf{Y})$  and show that

$$\mathbf{Y}(0) \text{ orthogonal} \implies \mathbf{Y}(t) \text{ orthogonal.}$$

(ii) [6 points] Consider the implicit mid-point method

$$\mathbf{Y}_{k+1} = \mathbf{Y}_k + \frac{\Delta t}{2} \mathbf{A}(\mathbf{Y}_k + \mathbf{Y}_{k+1}), \quad k = 0, \dots, K-1, \quad (1.2)$$

for solving (1.1) on  $[0, T]$  with the initial condition  $\mathbf{Y}_0 = \mathbf{Y}(0)$ . Here,  $\Delta t > 0$ ,  $K = T/\Delta t$ ,  $t_k = k\Delta t$  for  $k = 0, \dots, K$  and  $\mathbf{Y}_k = \mathbf{Y}(t_k)$ . We assume that  $K$  is an integer, for simplicity. Show that the solution  $\mathbf{Y}_k$  computed via the implicit mid-point method (1.2) satisfies

$$\mathbf{Y}_0 \text{ orthogonal} \implies \mathbf{Y}_k \text{ orthogonal for all } 1 \leq k \leq K.$$

HINT: Use the substitution  $\mathbf{Y}_{k+1} - \mathbf{Y}_k = \frac{\Delta t}{2} \mathbf{A}(\mathbf{Y}_k + \mathbf{Y}_{k+1})$  to show that  $2\mathbf{Y}_{k+1}^\top \mathbf{Y}_{k+1} - 2\mathbf{Y}_k^\top \mathbf{Y}_k = 0$ .

(1b) In addition to the implicit mid-point method, recall the explicit Euler method

$$\mathbf{Y}_{k+1} = \mathbf{Y}_k + \Delta t \mathbf{A} \mathbf{Y}_k \quad (1.3)$$

and the implicit Euler method

$$\mathbf{Y}_{k+1} = \mathbf{Y}_k + \Delta t \mathbf{A} \mathbf{Y}_{k+1}. \quad (1.4)$$

(i) **[8 points]** Complete the python templates `ExplEulStep.py`, `ImplEulStep.py` and `ImplMidpStep.py` to implement each of the explicit Euler method (1.3), the implicit Euler method (1.4) and the implicit mid-point method (1.2).

(ii) **[10 points]** Let  $n = 2$ ,  $\mathbf{A} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$  and  $\mathbf{Y}(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$ . Compute, using the three methods from part (1b)(i), discrete approximations  $\mathbf{Y}_k$  of  $\mathbf{Y}(t_k)$ , for  $k = 1, \dots, 20$  with  $\Delta t = 1/20$ . Compare the norms  $\|\mathbf{Y}_k^\top \mathbf{Y}_k - \mathbf{I}\|_F$ , for  $k = 1, \dots, 20$ . Briefly explain which methods you observe to preserve orthogonality, referring to the result from subproblem (1a)(ii).

HINT: The Frobenius norm  $\|\mathbf{M}\|_F$  of an  $m \times n$  matrix  $\mathbf{M}$  is defined as the square root of the sum of the absolute squares of its elements:

$$\|\mathbf{M}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n |m_{ij}|^2}. \quad (1.5)$$

It can be computed in Python using the command `linalg.norm(M, 'fro')` from the `numpy` library.

**Problem 2****[26 points]**Let  $\omega \in \mathbb{R}$ ,  $\omega \neq 0$ . Consider the system of equations

$$\begin{cases} \frac{dp}{dt} = -\omega q, & t \in [0, T], \\ \frac{dq}{dt} = \omega p, \\ p(t=0) = p_0 \in \mathbb{R}, \\ q(t=0) = q_0 \in \mathbb{R}. \end{cases} \quad (2.1)$$

**(2a)**

- (i) **[2 points]** Prove that (2.1) is a Hamiltonian system associated with the Hamiltonian function  $H(p, q) = \omega(p^2 + q^2)/2$ .
- (ii) **[3 points]** Prove that  $p^2 + q^2$  is an invariant of (2.1).

**(2b)** **[3 points]** Formulate the Leapfrog method (section 5.2.5 in the lecture notes) for (2.1).**(2c)** **[5 points]** Let  $\mathbf{y}(t) = (p(t), q(t))^\top$  and  $\mathbf{y}(t=0) = \mathbf{y}_0 = (p_0, q_0)^\top$ . Prove that

$$\mathbf{y}(t) = \mathbf{W}(t\omega)\mathbf{y}_0,$$

is the analytic solution to (2.1) with

$$\mathbf{W}(t\omega) := \exp\left(t \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix}\right).$$

Check that the eigenvalues of  $\mathbf{W}(t\omega)$  are  $\exp(\pm i \omega t)$ .**(2d)** **[4 points]** Transform the Leapfrog scheme from subproblem (2b) into the form

$$\mathbf{y}_{k+1} = \mathbf{S}(\Delta t \omega)\mathbf{y}_k,$$

with

$$\mathbf{S}(\Delta t \omega) = \begin{pmatrix} 1 - \frac{1}{2}(\Delta t \omega)^2 & -\Delta t \omega + \frac{1}{4}(\Delta t \omega)^3 \\ \Delta t \omega & 1 - \frac{1}{2}(\Delta t \omega)^2 \end{pmatrix},$$

which has the eigenvalues  $\lambda_{\pm} = \frac{1}{2}(2 - (\Delta t)^2 \omega^2 \pm \sqrt{(\Delta t)^4 \omega^4 - 4(\Delta t)^2 \omega^2})$ .**(2e)** **[9 points]** Implement the spectra of the exact and approximate evolution operators  $\mathbf{W}(\Delta t \omega)$  and  $\mathbf{S}(\Delta t \omega)$ . What do you observe for  $\Delta t \omega < 1$  and for  $\Delta t \rightarrow +\infty$ ? What can you deduce about the stability of the numerical method?

**Problem 3****[26 points]**

Let the continuously differentiable matrix-valued mapping  $\mathbf{A} : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d}$  satisfy

$$\mathbf{A}(\mathbf{y})^\top = -\mathbf{A}(\mathbf{y}) \quad \forall \mathbf{y} \in \mathbb{R}^d.$$

**(3a)** Let  $\mathbf{M} \in \mathbb{R}^{d \times d}$  be a  $d \times d$  matrix with real entries. We denote by  $\mathbf{M}^\top$  the transpose of  $\mathbf{M}$ . We say that  $\mathbf{M}$  is skew symmetric if  $\mathbf{M}^\top = -\mathbf{M}$ . We also say that a matrix  $\mathbf{B} \in \mathbb{R}^{d \times d}$  is orthogonal if  $\mathbf{B}\mathbf{B}^\top = \mathbf{I}$ , with  $\mathbf{I}$  being the  $d \times d$  identity matrix.

(i) **[2 points]** Prove that if  $\mathbf{M}$  is skew symmetric then  $\mathbf{M}x \cdot x = 0$  for all  $x \in \mathbb{R}^d$ .

(ii) **[2 points]** Prove that if  $\mathbf{M}$  is skew symmetric then  $e^{\mathbf{M}}$  is orthogonal.

**(3b)** **[2 points]** Show that the Euclidean vector norm  $\|\mathbf{y}\|$  is an invariant of every solution of the autonomous differential equation

$$\frac{d\mathbf{y}}{dt} = \mathbf{A}(\mathbf{y})\mathbf{y}. \quad (3.1)$$

HINT: Compute  $\frac{d}{dt} \|\mathbf{y}\|^2$ .

**(3c)** Consider the explicit Euler method,

$$\mathbf{y}_{k+1} = \mathbf{y}_k + \Delta t \mathbf{A}(\mathbf{y}_k) \mathbf{y}_k \quad (3.2)$$

the implicit Euler method

$$\mathbf{y}_{k+1} = \mathbf{y}_k + \Delta t \mathbf{A}(\mathbf{y}_{k+1}) \mathbf{y}_{k+1} \quad (3.3)$$

and the implicit single step method

$$\mathbf{y}_{k+1} = \mathbf{y}_k + \Delta t \mathbf{A}(\mathbf{y}_k + \mathbf{y}_{k+1})(\mathbf{y}_k + \mathbf{y}_{k+1}). \quad (3.4)$$

each applied to (3.1).

(i) **[2 points]** Show that  $\|\mathbf{y}_{k+1}\| \geq \|\mathbf{y}_k\|$  for the explicit Euler method (3.2) applied to (3.1).

(ii) **[2 points]** Show that  $\|\mathbf{y}_{k+1}\| \leq \|\mathbf{y}_k\|$  for the implicit Euler method (3.3) applied to (3.1).

(iii) **[2 points]** Show that  $\|\mathbf{y}_{k+1}\| = \|\mathbf{y}_k\|$  for the implicit single step method (3.4) applied to (3.1).

**(3d)** Consider now the explicit exponential single step method defined by

$$\begin{aligned} \mathbf{y}_{k+\frac{1}{2}} &= \mathbf{y}_k + \frac{1}{2}\Delta t \mathbf{A}(\mathbf{y}_k) \mathbf{y}_k, \\ \mathbf{y}_{k+1} &= \exp(\Delta t \mathbf{A}(\mathbf{y}_{k+\frac{1}{2}})) \mathbf{y}_k. \end{aligned} \tag{3.5}$$

(i) **[2 points]** Show that  $\|\mathbf{y}_{k+1}\| = \|\mathbf{y}_k\|$  for (3.5).

HINT: Use the result from subproblem (3a)(i).

(ii) **[4 points]** Prove that, provided  $t \mapsto \mathbf{y}(t)$  is smooth enough,

$$\mathbf{y}(t+\Delta t) = \mathbf{y}(t) + \Delta t \mathbf{A}(\mathbf{y}(t)) \mathbf{y}(t) + \frac{(\Delta t)^2}{2} [\nabla \mathbf{A}(\mathbf{y}(t)) (\mathbf{A}(\mathbf{y}) \mathbf{y}, \mathbf{y}) + \mathbf{A}(\mathbf{y}(t))^2 \mathbf{y}(t)] + \mathcal{O}((\Delta t)^3)$$

HINT: Use a Taylor expansion.

(iii) **[1 point]** Rewrite (3.5) in the form

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

with  $\Phi(t, \mathbf{y}, \Delta t)$  defined by

$$\Phi(t, \mathbf{y}, \Delta t) = \frac{1}{\Delta t} \left( \exp \left( \Delta t \mathbf{A} \left( \mathbf{y} + \frac{\Delta t}{2} \mathbf{A}(\mathbf{y}) \mathbf{y} \right) \right) - \mathbf{I} \right) \mathbf{y}$$

(iv) **[5 points]** Deduce that the truncation error

$$T_k(\Delta t) := \frac{\mathbf{y}(t_{k+1}) - \mathbf{y}(t_k)}{\Delta t} - \Phi(t_k, \mathbf{y}(t_k), \Delta t)$$

is of order  $\mathcal{O}((\Delta t)^2)$  as  $\Delta t \rightarrow 0$  and therefore, the explicit exponential single step scheme is consistent and is of order at least 2.

**(3e) [2 points]** Suppose that  $\mathbf{A}(\mathbf{y}) = \mathbf{A}$ , a constant skew-symmetric matrix, for all  $\mathbf{y} \in \mathbb{R}^d$ . Show that (3.5) yields the exact solution in this case.