Numerical Analysis II

Problem Sheet 14

Problem 14.1 ODEs for Matrix-Valued Functions

Let the matrix-valued function $\mathbf{Y} : \mathbb{R} \to \mathbb{R}^{d \times d}$ be a solution of the (matrix) differential equation

$$\dot{\mathbf{Y}} = \mathbf{A}\mathbf{Y} \quad \text{with} \quad \mathbf{A} \in \mathbb{R}^{d \times d}. \tag{14.1.1}$$

(14.1a) Assume $\mathbf{A}^\top \mathbf{H} = -\mathbf{H}\mathbf{A}$. Show that $\mathbf{Y}(t)^\top \mathbf{H}\mathbf{Y}(t) = \mathbf{H}$ for all $t > 0$ provided $\mathbf{Y}(0)^\top \mathbf{H}\mathbf{Y}(0) = \mathbf{H}$.

HINT: You might want to compute $\frac{\mathrm{d}}{\mathrm{d}t}$ of $\mathbf{Y}^\top \mathbf{H}\mathbf{Y}$.

(14.1b) Implement the following functions in MATLAB

(i) `function Y = ExplEulStep(A, Y0, h)`,

(ii) `function Y = ImplEulStep(A, Y0, h)`,

(iii) `function Y = ImplMidpStep(A, Y0, h)`,

which, for a given initial value $\mathbf{Y}(t_0) = \mathbf{Y}_0$ and for a given step size h, compute approximations to $\mathbf{Y}(t_0 + h)$ for the solution of (14.1.1) using a (*single*) step of

(i) the explicit Euler method,

(ii) the implicit Euler method,

(iii) the implicit mid-point method.

(14.1c) Take now $\mathbf{A} = \begin{pmatrix} -3 & -6 \\ 6 & 3 \end{pmatrix}$, $\mathbf{Y}(0) = \frac{1}{\sqrt{3}} \begin{pmatrix} 2 & 1 \\ -1 & -2 \end{pmatrix}$, and $\mathbf{H} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$. Complete the template `CompareNorms.m` where, using the functions from subproblem (14.1b), you should compute discrete approximations $\mathbf{Y}_k$ of $\mathbf{Y}(kh)$, for $k = 1, \ldots, 20$ with $h = 1/20$. Compare the norms $\left\| \mathbf{Y}_k^\top \mathbf{H}\mathbf{Y}_k - \mathbf{H} \right\|_F$, for $k = 1, \ldots, 20$ and all three methods, and comment on your observations with regards to the invariant from subproblem (14.1a).

HINT: The Frobenius norm $\|\cdot\|_F$ of a matrix can be computed using the command `norm(A,'fro')`.

(14.1d) Show that the solution $\mathbf{Y}_k$ computed via the implicit mid-point rule satisfies:

$$\text{if} \quad \mathbf{Y}_0^\top \mathbf{H}\mathbf{Y}_0 = \mathbf{H} \quad \text{then} \quad \mathbf{Y}_k^\top \mathbf{H}\mathbf{Y}_k = \mathbf{H} \quad \text{for all } k \geq 1.$$

HINT: You might find the identity $\mathbf{Y}_1 - \mathbf{Y}_0 = \frac{h}{2}\mathbf{A}(\mathbf{Y}_0 + \mathbf{Y}_1)$ useful.

Problem 14.2 Projection Method for Hamiltonian equations

When an ODE is defined on a manifold it is important that the approximate solution is also contained in the manifold. A natural ansatz consists in projecting the approximate solution to this manifold. In the present exercise we will apply this ansatz to Hamilton's equations in such a way that important first integrals are preserved. We will also investigate how many such projections are necessary in order to obtain a qualitatively correct solution.

As our example we consider the perturbed Kepler problem whose Hamiltonian is given by

$$H(\mathbf{p},\mathbf{q}) = \frac{1}{2}\left(p_1^2 + p_2^2\right) - \frac{1}{\sqrt{q_1^2+q_2^2}} - \frac{0.005}{2\sqrt{\left(q_1^2+q_2^2\right)^3}}. \tag{14.2.1}$$

(14.2a) Derive the Hamilton's equations for (14.2.1).

(14.2b) Write down a first integral for the ODE derived in subproblem (14.2a) and show that the angular momentum

$$L(\mathbf{p},\mathbf{q}) = q_1 p_2 - q_2 p_1 \tag{14.2.2}$$

defines an additional first integral.

(14.2c) Fill in the template `proHam1.m` which solves the ODE 14.2.1 using the explicit Euler method, the Störmer–Verlet method and the symplectic Euler method and plots the trajectory of the position coordinate $\binom{q_1(t)}{q_2(t)}$ for each of the three aforementioned methods .

HINT: The symplectic Euler method is a Lie–Trotter splitting method, see [NUMODE, Eq. (2.5.11)].

(14.2d) subproblem (14.2c) makes clear the fact that the explicit Euler method yields a qualitatively wrong solution. To obtain a better approximation, we project the numerical solution to the submanifold

$$\mathcal{M} := \left\{ \mathbf{z} = \begin{pmatrix}\mathbf{x}\\ \mathbf{y}\end{pmatrix} \in \mathbb{R}^4 \;\middle|\; H(\mathbf{x},\mathbf{y}) = H(\mathbf{p}(0),\mathbf{q}(0)) \right\} \subseteq \mathbb{R}^4$$

after each time step. Let $\mathbf{z} \in \mathbb{R}^4$ (e.g. $\mathbf{z}$ might represent the approximation computed using the explicit Euler method). A projection $\tilde{\mathbf{z}}$ of $\mathbf{z}$ onto the manifold $\mathcal{M}$ can be defined to be a solution of the following system

$$\begin{aligned} \tilde{\mathbf{z}} &= \mathbf{z} + s\,\mathbf{grad}(H(\mathbf{z})), \\ 0 &= H(\tilde{\mathbf{z}}) - H(\mathbf{p}(0),\mathbf{q}(0)), \end{aligned} \tag{14.2.3}$$

where $s \in \mathbb{R}$. Carry out one step of the Newton method for (14.2.3) and determine an approximation of the projection $\tilde{\mathbf{z}}$. Choose $s^{(0)} = 0$ as the initial value for the parameter s.

HINT: Solve (14.2.3) for s as the only unknown. Then determine an approximation for s via the Newton method and construct the projection $\tilde{\mathbf{z}}$.

(14.2e) Complete the template `proHam2.m`, which solves the ODE (14.2.1) using the method derived in subproblem (14.2d), and plots the trajectory of the position coordinates $\binom{p_1(t)}{p_2(t)}$ as well as the evolution of the energy.

(14.2f) From the subproblem (14.2e) we can infer that the projection to the manifold $\mathcal{M}$ is not sufficient to obtain a qualitatively correct solution. Let us try to improve this method by projecting onto a smaller submanifold of $\mathbb{R}^4$, given by

$$\mathcal{L} := \left\{ \mathbf{z} = \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} \in \mathbb{R}^4 \,\middle|\, H(\mathbf{x}, \mathbf{y}) = H(\mathbf{p}(0), \mathbf{q}(0)),\ L(\mathbf{x}, \mathbf{y}) = L(\mathbf{p}(0), \mathbf{q}(0)) \right\}.$$

The projection $\tilde{\mathbf{z}}$ of $\mathbf{z}$ to the manifold $\mathcal{L}$ can be defined as the solution to the following system

$$\begin{aligned} \tilde{\mathbf{z}} &= \mathbf{z} + s\,\mathbf{grad}(H(\mathbf{z})) + r\,\mathbf{grad}(L(\mathbf{z})), \\ 0 &= H(\tilde{\mathbf{z}}) - H(\mathbf{p}(0), \mathbf{q}(0)), \\ 0 &= L(\tilde{\mathbf{z}}) - L(\mathbf{p}(0), \mathbf{q}(0)), \end{aligned} \tag{14.2.4}$$

where s and r are real parameters. Carry out one step of the Newton method for (14.2.4) and compute an approximation of the projection $\tilde{\mathbf{z}}$. Choose $s^{(0)} = 0$ and $r^{(0)} = 0$ as starting values for s and r.

HINT: Solve (14.2.3) for s and r as the only unknowns. Then determine an approximation for s and r via the Newton method and construct the projection $\tilde{\mathbf{z}}$.

(14.2g) Complete the template `proHam3.m` which solves the ODE (14.2.1), using the method described in subproblem (14.2f), and plots the trajectory of the position coordinates $\binom{p_1(t)}{p_2(t)}$ as well as the evolution of the energy and the angular momentum.

Problem 14.3 Instability of the Störmer-Verlet Method

We consider the Hamiltonian of a harmonic oscillator, with a frequency parameter $\omega \in \mathbb{R}$, defined as

$$H(p, q) = \frac{1}{2}\omega(p^2 + q^2), \quad p, q \in \mathbb{R}.$$

(14.3a) Formulate the corresponding Hamilton's equations.

(14.3b) Formulate the Störmer-Verlet method for the ODE from subproblem (14.3a).

(14.3c) The analytic solution $\mathbf{y}(t) := (p(t), q(t))^\top$ of the ODE from subproblem (14.3a) is

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

with

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

Plot the eigenvalue loci of $\mathbf{W}(t\,\omega)$, with respect to $t\,\omega$.

(14.3d) Transform the Störmer-Verlet method obtained in subproblem (14.3b) into the form

$$\mathbf{y}_1 = \mathbf{S}(h\,\omega)\mathbf{y}_0.$$

Plot the eigenvalue loci, with respect to $h\omega$. What can you observe by comparing this curve with the curve obtained in subproblem (14.3c)?

(14.3e) What do you observe for $h\omega \to \infty$? What are the consequences on the numerical method?

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There's no submission deadline for this assignment, but at least having a look at all assignments before final exam might be a good suggestion.

References

[NODE] Lecture Notes for the course "Numerical Methods for Ordinary Differential Equations".

[NUMODE] Lecture Slides for the course "Numerical Methods for Ordinary Differential Equations", SVN revision # 52913.

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