Homework 5
APPM 4720/5720 Scientific Machine Learning, Fall 2024

Due date: Monday, Sep. 30 '24, before midnight, via Gradescope

Instructor: Prof. Becker
Revision date: 9/30/2024

Theme: ODE solvers (for a Hamiltonian system)

Instructions Collaboration with your fellow students is OK and in fact recommended, although direct copying is not allowed. The internet **is allowed for basic tasks** (e.g., looking up definitions on wikipedia, looking at documentation, looking at basic tutorials) but it is not permissible to search for solutions to the exact problem or to *post* requests for help on forums such as `http://math.stackexchange.com/`.

Background The **two-body problem** is about predicting the motion of two objects orbiting each other in space, interacting with each other (due to gravity). It can be reduced to a pair of one-body problems and what's left is the Kepler problem, as we'll describe below. This has a long history, and for many years people tried to have similarly clean analysis of the three-body problem but without luck (now known to be generally impossible, though numerically it's not an issue).

For us, we have a variable $\mathbf{x} \in \mathbb{R}^2$ and its corresponding velocity $\mathbf{v} \in \mathbb{R}^2$ (note: even if we work in 3D, all the motion will stay in a fixed plane, so we can still work in 2D without loss of generality), and assuming the center of mass is at the origin, we have a coupled 4D system of ODEs:

$$\begin{aligned}\frac{d\mathbf{x}}{dt} &= \mathbf{v}(t)\\ \frac{d\mathbf{v}}{dt} &= -\mu\frac{\mathbf{x}(t)}{\|\mathbf{x}(t)\|^3}\end{aligned} \tag{Kepler problem}$$

where $\mu = 4\pi^2$ (we have used non-dimensionalized units; we will interpret time as being in units of years, and you can think of a distance of 1 being one astronomical unit). Use starting conditions $\mathbf{x}(0) = [1, 0]$ and $\mathbf{v}(0) = [0, 1.1\sqrt{\mu}]$. This should lead to elliptical orbits (if we had used $\mathbf{v}(0) = [0, \sqrt{\mu}]$ it would be perfectly circular) of period close to 1. We could find a closed form solution (see wikipedia), but for now the main analytic observation is that the force is conservative (there is no friction nor drag) and therefore total energy is conserved. *Recall total energy is potential plus kinetic, with potential being* $-\mu/\|\mathbf{x}\|$ *and kinetic being* $\frac{1}{2}\|\mathbf{v}\|^2$.

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Problem 1: Write ODE solvers for the Kepler problem using at least 2 methods: forward Euler, and a symplectic method (e.g., Semi-implicit Euler method (also known as symplectic Euler, semi-explicit Euler, Euler–Cromer, and Newton–Størmer–Verlet (NSV)), or velocity Verlet). $\boxed{\text{Turn in the code in a nice PDF}}$.

Students in 5720 must also implement a third method: backward Euler. *For backward Euler, you have at least three implementation options. You can solve iteratively via Picard iterations, or iteratively via Newton-Raphson, or solve it (mostly) by hand.*

Problem 2: Simulate the system for 10 years using all two (or three) solvers you created, with a timestep Δt being a quarter of a day (remember, time is in units of years). $\boxed{\text{Plot the total energy}}$ as a function of time for all two (or three) methods. $\boxed{\text{Make some observations}}$ about conservation of energy.

Problem 3: **Refinement study**. Take an even smaller time step Δt and solve the ODE; we'll take this as a "ground truth". Then solve the ODE using progressively larger stepsizes (I'd suggest increasing them by a factor of 2 every time), and look at the error compared to the "ground truth" in terms of the mean-squared-error of all the state variables (that is, $\mathbf{x}$ and $\mathbf{v}$) *(When doing this, don't forget to subset as needed, so that you are matching the right time points)*. Repeat this for all two (or three) methods, and turn in a log-log $\boxed{\text{plot of stepsize vs error}}$, and $\boxed{\text{comment on what you think the order of each method is}}$. **You only need to do this for a time range of 1 year**.

Problem 4: For at least one of the methods, plot the total energy for a variety of stepsizes, and $\boxed{\text{comment on whether refining the stepsize helps conservation of energy}}$.

Problem 5: **Students in 5720 only** Back to using Δt being a quarter of a day, run the backward Euler method for 11.5 years and $\boxed{\text{comment on what you observe}}$ and discuss $\boxed{\text{possible explanations}}$.