Homework 8

Math 651
Fall 2019

Due Friday, November 22, 2019

Consider Newton's equations

$$x' = v, \text{ and}$$
$$v' = -\nabla V(x)$$

for some *potential energy* $V : \mathbb{R}^d \to \mathbb{R}$. (Here, $x : [0, \infty) \to \mathbb{R}^d$, $v : [0, \infty) \to \mathbb{R}^d$.) Newton's equations model the motion of the planets, the vibrations of molecules, and many other phenomena. The simplest example of a system governed by Newton's equations is the *harmonic oscillator*

$$\begin{cases} x' = v, \text{ and} \\ v' = -x, \end{cases}$$

for which the potential energy is

$$V(x) = \frac{1}{2}x^2.$$

Problem 1 (2+2+2 points)**.**

1. *Let x and v solve Newton's equations with potential energy V. Define the* Hamiltonian
$$H(x, v) = \frac{1}{2}|v|^2 + V(x).$$
Show that $H(x(t), v(t)) = H(x(0), v(0))$ for all $t > 0$. This property is of extreme importance in physics: it is called conservation of energy.

   Hint: *What is $\frac{d}{dt}H(x(t), v(t))$ when x and v solve Newton's equations?*

2. *Use Euler's method to solve the initial value problem for the harmonic oscillator with $x_0 = 1$ and $v_0 = 0$. Compute the numerical solution up to time $T = 30$ using the time step $\Delta t = 0.02$. Plot the numerical solution (x_n, v_n) as a curve in the xv plane. You should see a spiral. Plot the Hamiltonian as a function of time for the numerical solution. Observe that the Hamiltonian is* not *conserved for Euler's method!*

3. *Define the* Störmer–Verlet Method

$$
\begin{aligned}
v_{n+\frac{1}{2}} &= v_n - \frac{1}{2}\Delta t \nabla V(x_n) \\
x_{n+1} &= x_n + \Delta t v_{n+\frac{1}{2}} \\
v_{n+1} &= v_{n+\frac{1}{2}} - \frac{1}{2}\Delta t \nabla V(x_{n+1}).
\end{aligned}
$$

Observe that Störmer–Verlet is similar to Euler's Method, except that the update of the variable v is split into two pieces. Use Störmer–Verlet to solve the initial value problem for the harmonic oscillator with $x_0 = 1$ and $v_0 = 0$. Compute the numerical solution up to time $T = 30$ using the time step $\Delta t = 0.02$. Make the same plots as for Euler's method. Observe that the Hamiltonian is nearly conserved.

Remark 1. The Störmer–Verlet Method is a *symplectic integrator*. Symplectic integrators preserve certain geometric properties of Newton's equations. In general, for symplectic integrators, the Hamiltonian is not exactly constant over trajectories, but one can show that a slightly perturbed version of the Hamiltonian is very nearly constant. No such property holds for Euler's method.

Problem 2 (3 points)**.** *Recall that the trapezoidal rule is the numerical integrator defined by*

$$x_{n+1} = x_n + \frac{\Delta t}{2}(f(x_n, n\Delta t) + f(x_{n+1}, (n+1)\Delta t))).$$

Find the linear stability domain of the trapezoidal rule.

Problem 3 (2+2+4+2 points)**.** *Recall that the implicit Euler method is the numerical integrator defined by*

$$x_{n+1} = x_n + \Delta t f(x_{n+1}, (n+1)\Delta t).$$

Assume that the right-hand-side $f : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}^n$ of the initial value problem is globally Lipschitz with constant L. That is,

$$\|f(x,t) - f(y,t)\| \leq L\|x - y\|$$

for all $x, y \in \mathbb{R}^n$. Let $T > 0$. Assume that $\Delta t L \leq \frac{1}{2}$.

1. *Prove that the implicit Euler method is consistent of order one. That is, show that for any $t \in [0, T - \Delta t]$,*

   $$\|x(t+\Delta t) - x(t) - \Delta t f(x(t+\Delta t), t+\Delta t)\| \leq C\Delta t^2,$$

   where $x(t)$ is the exact solution of the IVP and C is some constant that may depend on $x(t)$ but that does not depend on Δt. You may assume without comment that $x(t)$ is twice continuously differentiable.

2. *To assist in your proof of stability below, show that whenever* $\Delta t L \leq \frac{1}{2}$*, we have*

$$\frac{1}{1 - \Delta t L} \leq \exp\left(2L\Delta t\right).$$

3. *Prove that the implicit Euler method is stable. To be more precise, suppose that* y_n *solves*

$$y_{n+1} = y_n + \Delta t f(y_{n+1}, (n+1)\Delta t) + G_n,$$

where $\|G_n\| \leq \varepsilon$*. Show that*

$$\max_{n=0,\ldots,\lfloor \frac{T}{\Delta t} \rfloor} \|y_n - x_n\| \leq \frac{\varepsilon}{\Delta t L} \exp\left(2LT\right).$$

4. *Prove that the implicit Euler method is convergent of order one. That is, show*

$$\max_{n=0,\ldots,\lfloor \frac{T}{\Delta t} \rfloor} \|x_n - x(n\Delta t)\| \leq D\Delta t \exp\left(2LT\right)$$

for some constant D *that may depend on the exact solution* $x(t)$ *of the IVP but that does not depend on* Δt*.*

Problem 4 (5 points)**.** *Let* $f \in C([0,1])$*, and let* $u \in C^2([0,1])$ *be a solution of the boundary value problem*

$$\begin{cases} u''(x) = f(x) & \text{for } x \in (0,1), \\ u(0) = 0, \\ u(1) = 0. \end{cases}$$

Show that

$$\|u\|_\infty \leq \frac{1}{8}\|f\|_\infty.$$

Hint: *Mimic the argument for the discrete analogue of this result. Use the comparison function*

$$\phi(x) := \frac{1}{2}\left(x - \frac{1}{2}\right)^2.$$

Problem 5 (2+1+2 points)**.** *Define the forwards finite difference operator* $D_{\Delta x} : \mathbb{R}^{N-1} \to \mathbb{R}^{N-1}$ *by*

$$(Dv)_i = \frac{v_{i+1} - v_i}{\Delta x} \text{ for } i = 1, \ldots, N-1.$$

When $i = N-1$ *above, we set* $v_N = 0$*. Recall that we adopted a similar convention in defining the discrete Laplacian* Δ_{Δ_x}*.*

1. *Define the backwards difference*

$$(D^-_{\Delta x} v)_i := \frac{v_i - v_{i-1}}{\Delta x} \text{ for } i = 1, \dots, N-1,$$

where again we take $v_0 = 0$. *Show that* $-D^{\mathrm{t}}_{\Delta x} = D^-_{\Delta x}$.

Hint: *The right way to do this is to show* $\langle D_{\Delta x} u, v\rangle = -\langle u, D^-_{\Delta x} v\rangle$ *for all* $u, v \in \mathbb{R}^{N-1}$. *You don't ever have to explicitly write the difference operator as a matrix, and that makes everything easier.*

2. *What does the above have to do with integration by parts?*

3. *Show that* $\Delta_{\Delta x} = -D^{\mathrm{t}}_{\Delta x} D_{\Delta x}$.

Hint: *Again, the right way is to show that* $\langle \Delta_{\Delta x} u, v\rangle = -\langle D_{\Delta x} u, D_{\Delta x} v\rangle$. *You shouldn't ever have to explicitly write down and multiply matrices.*

The problem above will be continued next week—you'll see the point eventually.