Lecture 8 2/24

- Nonlinear learnable stencil
- Multi-step/stage integrators
- Linear stability analysis
- Störmer-Verlet

Let's recall what we know now how to do

- Use least action to derive an energy/momentum preserving ODE
- Use Legendre ~~Noether~~ to compute a Hamiltonian
- Use discrete gradient to integrate (example to come)
- Use Pytorch to solve for nonlinear stencils
- Use polynomial reproduction + Noether to put constraints on stencil

With these in hand, we are ready to assume our final form.... nonlinear wave eqn solver!

1D Wave Eqn in Periodic BC

$$\begin{cases} \partial_{tt} u = c^2 \partial_{xx} u \\ u(x,t=0) = f(x) \end{cases}$$

Soln given by $u(x,t) = f(x+ct) + f(x-ct)$

To confirm

$$\partial_{xx} u = f''(x+ct) + f(x-ct)$$
$$\partial_t u = c f'(x+ct) - c f(x-ct)$$
$$\partial_{tt} u = c^2 f''(x+ct) + c^2 f(x-ct) \quad \checkmark$$

We will derive an architecture that can recover this simple case

- In previous class, we saw that in the absence of the right most node $\left(D_h u^2 = D_- u^2\right)$ the Lagrangian yields the approximation $\left(\nabla^2 u \approx D_h^* D_h u = D_+ D_- u\right)$.

Goal as expressive an ansatz as possible while satisfying constraints

- Motivated by this, we will hypothesize

$$S = \underbrace{\sum_i \frac{1}{2} \dot{q}_i^2 h}_{S_1} - \underbrace{\frac{1}{2} N(D_- q; \theta)^2 h}_{S_2}$$

- Note that this is shift invariant for q and t
- here there were some options - we could also have explored e.g. $D_- N(q;\theta)$, or $D_- q \to \alpha q_{i-1} - \alpha q_i$ for any α
- variations of the first term give $\delta_q S_1 = -\ddot{q}_i h$

for second term

$$\left(\delta_q S_2, \delta q\right) = \lim_{\varepsilon \to 0} \int_{t_0}^{t} \frac{1}{2} \frac{1}{\varepsilon} \left[N\left(D_-(q+\varepsilon \delta q); \theta\right) - N(D_- q; \theta)\right] dt$$

def of directional derivative

$$= \lim_{\varepsilon \to 0} \int_{t_0}^{t} \frac{1}{2} \frac{1}{\varepsilon} \nabla N\left(D_-(q+\varepsilon\delta q); \theta\right) \cdot D_-(\varepsilon \delta q) \, dt$$

$$= \int_{t_0}^{t} \nabla N(D_- q) \cdot D_- \delta q \, dt$$

$$= \int_{t_0}^{t} \underbrace{D_+ \nabla N(D_- q)}_{\delta_q S_2} \delta q \, dt$$

And we obtain the dynamics

$$\ddot{q}_i = D_+ \nabla N(D_- q; \theta)$$

We can identify the generalized momentum

~~$p(x,t) =$~~

$$p_i(t) = \partial_{\dot{q}_i} L = \dot{q}_i h$$

Applying the Legendre transform

$$H = p \cdot \dot{q} - L$$

$$= \sum_i \dot{q}_i^2 h - \frac{1}{2} \dot{q}_i^2 h - \frac{1}{2} N(D-q;\theta)^2 h$$

$$= \sum_i \frac{1}{2} \dot{q}_i^2 h + \frac{1}{2} N(D-q;\theta)^2 h$$

$$= \underbrace{\sum_i \frac{1}{2} p_i^2 h^{-1}}_{\underbrace{T_\theta(p)}_{\text{kinetic}}} + \underbrace{\frac{1}{2} N(D-q;\theta)^2 h}_{\underbrace{V_\theta(q)}_{\text{potential}}}$$

Want to solve

$$\boxed{\begin{aligned} \frac{dp}{dt} &= -\partial_q V_\theta(q) \\ \frac{dq}{dt} &= \partial_p T_\theta(p) \end{aligned}}$$

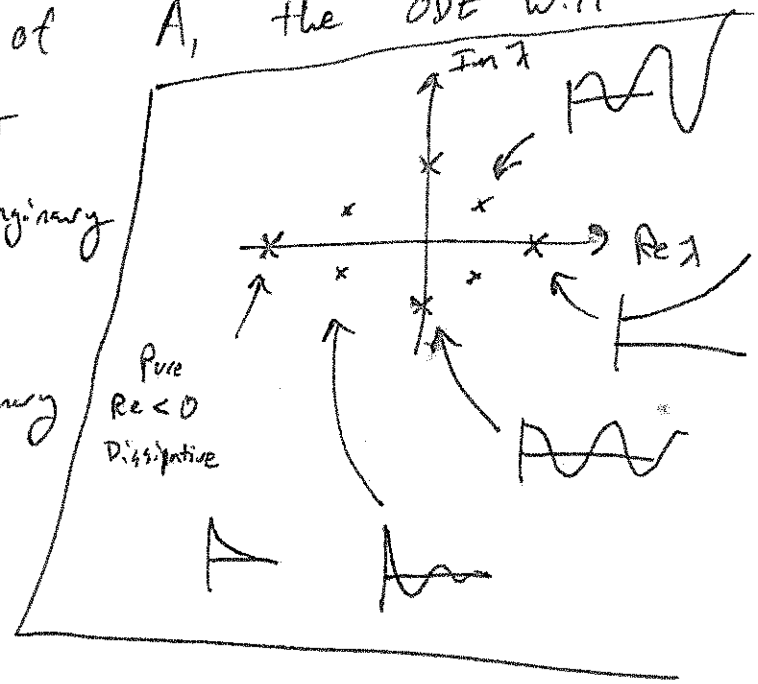
Some final remarks on time integration

To choose an integration scheme (so far we only looked at explicit Euler)

Consider a linear system of ODEs

$$\dot{y} = Ay$$

- Depending on the eigenvalues of A, the ODE will have distinct character
- Hyperbolic PDE corresponds to purely imaginary
- We'll next cover some options that can handle purely imaginary eigenvalues



Time Integration

Consider now non-linear $\dot{x} = F(x;\theta)$

Two broad classes for explicit methods ← why is explicit important for ML?

Multi-stage schemes

$$x^{n+1} = x^n + \overset{\text{timestep}}{h} \sum_{i=1}^{s} b_i \overset{\text{stage}}{K_i}$$

$$K_i = F\left(t_n + c_i h,\ x^n + h \sum_{j=1}^{i-1} a_{ij} K_j\right)$$

<u>idea</u> at each stage you can make an additional gradient evaluation using points generated in previous stages

Multi-step schemes

$$\sum_{j=0}^{s} a_j x^{n+1-j} = h \sum_{j=0}^{s-1} b_j f(t_{n-j}, x_{n-j})$$

- $a_0 = 1$
- if $a_j = 0$ for $j > 0$, scheme is explicit
- <u>idea</u> use information about derivative from previous timestep to predict

<u>Comparison</u>
- Multi-step only needs 1 func eval per step ⇒ generally faster
- Complicated for first s steps, need to start up w/ multistage
- For simplicity we'll just use multistage

Examples

RK1 - explicit Euler

$$K_1 = F(t_n, x_n)$$

$$x_{n+1} = x_n + h K_1$$

2^{nd} order schemes

After E.E. for stage 1, make ansatz

$$K_2 = F(t_n + \alpha h,\ x_n + \beta K_1)$$

$$x_{n+1} = x_n + h(a K_1 + b K_2)$$

To choose, expand in Taylor series

$$F(t_n + \alpha h,\ x_n + \beta K_1)$$

because $K_1 = F(t_n, x_n)$

$$= F(t_n, x_n) + \partial_t F(t_n, x_n)\, \alpha h + \partial_x F(t_n, x_n)^2 \beta \Delta t$$

And so

denote $F_n = F(t_n, x_n)$

$$x_{n+1} = x_n + h(a K_1 + b K_2)$$

$$= x_n + h a F_n + h b F_n + \alpha b h^2 \partial_t F_n + \beta b h^2 \partial_x F_n$$

$$= x_n + h(a+b) F_n + \tfrac{1}{2} h^2 (2\alpha b)\, \partial_t F_n + \tfrac{1}{2} h^2 (2\beta b)\, \partial_x F_n$$

Compare to linear terms in T.S expansion

$$\boxed{\begin{aligned} a + b &= 1 \\ \alpha b &= 1/2 \\ \beta b &= 1/2 \end{aligned}}$$

$\leftarrow$ Non-unique!

~~Examples~~

RK2 take $a = b = 1/2$

$\alpha = \beta = 1$

AKA How to read off wikipedia

For the general scheme

$$x_{n+1} = x_n + h \sum_{i=1}^{s} b_i K_i$$

$$K_i = F\left(t_n + hc_i,\ x_n + h \sum_{j=1}^{i-1} a_{ij} K_j\right)$$

Coefficients are written compactly as a Butcher tableau

$$\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \cdots & - \\
c_2 & a_{21} & & & \\
\vdots & \vdots & \ddots & & \\
c_s & & & & \\
\hline
 & b_1 & b_2 & \cdots & b_s
\end{array}$$

First order methods

$$\begin{array}{c|c}
0 & 0 \\
\hline
 & 1
\end{array}$$

Only one choice → our friend E.E.

2nd order methods

$$\begin{array}{c|cc}
0 & 0 & 0 \\
\alpha & \alpha & 0 \\
\hline
 & \left(1 - \frac{1}{2\alpha}\right) & \frac{1}{2\alpha}
\end{array}$$

for any α

Notable examples

$\alpha = \frac{1}{2}$ explicit midpt

$\alpha = 1$ Heun

$\alpha = 2/3$ Ralston

3rd order

$$\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
\alpha & \alpha & 0 & 0 \\
\beta & \left(\frac{\beta}{\alpha}\ \frac{\beta - 3\alpha(1-\alpha)}{3\alpha - 2}\right) & \left(-\frac{\beta}{\alpha}\ \frac{\beta-\alpha}{(3\alpha-2)}\right) & 0 \\
\hline
 & 1 - \frac{3\alpha + 3\beta - 2}{6\alpha\beta} & \frac{3\beta - 2}{6\alpha(\beta-\alpha)} & \frac{2 - 3\alpha}{6\beta(\beta-\alpha)}
\end{array}$$

Note

At this pt we should get excited when we see parameterized schemes like this!

4th order

Standard RK4

0	0	0	0	0
1/2	1/2	0	0	0
1/2	0	1/2	0	0
1	0	0	1	0
	1/6	1/3	1/3	1/6

To understand why this is the default, we need to analyze the stability. We'll see this works for purely imaginary problems

Linear Stability of multi-stage schemes

Consider again $\dot{y} = Ay$

Lets analyze RK2

$$y_{n+1} = y_n + \frac{h}{2}(K_1 + K_2)$$

$$K_1 = Ay_n$$

$$K_2 = F(t_n + h, y_n + hK_1)$$

$$= A(y_n + hK_1)$$

$$= Ay_n + hA^2 y_n$$

So $$y_{n+1} = \underbrace{\left(I + hA + \frac{h^2}{2}A^2 \right)}_{Q} y_n$$

amplification factor

Note what drives the choices of coeffs in RK is that $Q \approx \exp(A)$

Thm

Consider an arbitrary scheme, where Q is ~~non singular~~ diagonalizable

$$y_{now} = Q^n y_0$$

Then if λ_i is the ~~max~~ i^{th} eigenvalue of Q

$$\max_i |\lambda_i| \leq 1 \Rightarrow \|y_{n+1}\| \leq \|y_0\|$$

Pf Nonsingular $\Rightarrow Q = S \Lambda S^{-1}$, $\Lambda = \operatorname{diag}(\lambda_1, \dots \lambda_N)$

$$y_n = (S\Lambda S^{-1})(S\Lambda S^{-1}) \cdots \overset{n \text{ times}}{\cdots} (S\Lambda S^{-1}) y_0$$

$$= S \Lambda^n S^{-1} y_0$$

$$S^{-1} y_n = \Lambda^n S^{-1} y_0$$

Or if $w_n = S^{-1} y_n$

$$w_n = \Lambda^n w_0$$

Componentwise

$$w_{n,i} = \lambda_i^n w_{0,i}$$

Which is bnded if $\max \lambda_i \leq 1$

- How does this translate to RK2?

- Recall <u>def</u> spectral radius

$$\rho(A) = \max\{ |\lambda_i| ,\ \lambda_i \text{ is e.g. of } A \}$$

- Want

$$\rho(Q) = 1 + h\rho(A) + \frac{h^2}{2}\rho(A)^2 \quad \text{to be} \leq 1$$

Let $z = h\rho(A) \in \mathbb{C}$ ← complex #'s

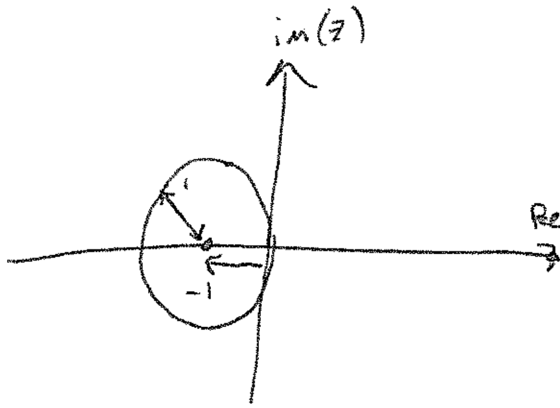
Solve for z s.t.

$$g(z) = 1 + z + \frac{1}{2}z^2 \leq 1$$

- In general gnarly to do by hand. Simple to meshgrid in matplotlib

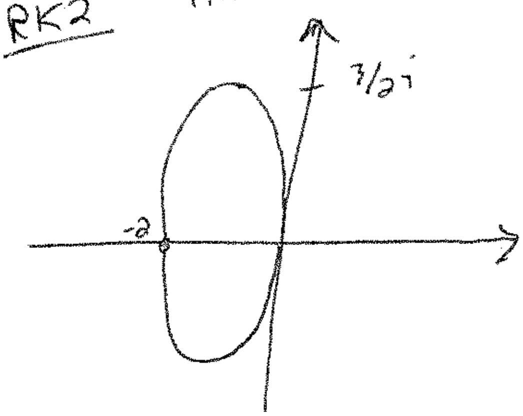
RK1

we already saw this only works w/ stabilization

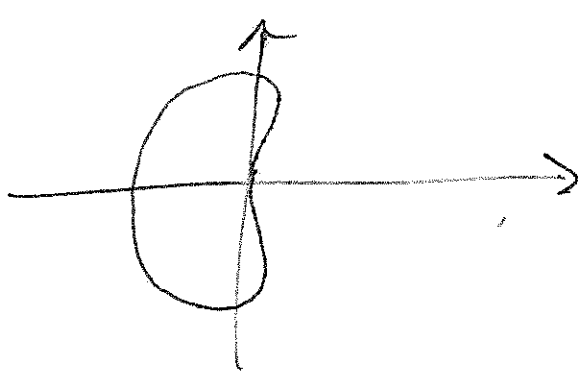


RK2

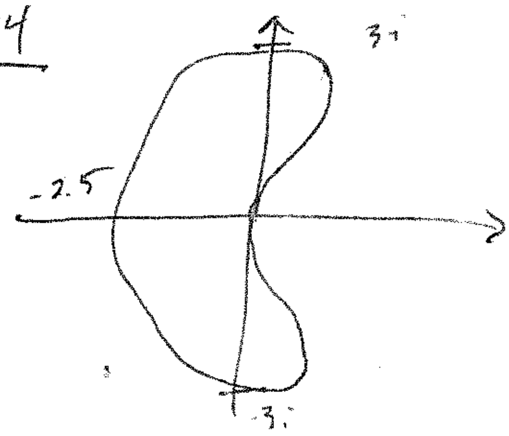
stretch by 3/2 in im part



RK3



RK4



Symplectic Integrators

Recall that for a canonical Hamiltonian system

$$\dot{p} = -\partial_q H$$
$$\dot{q} = \partial_p H \quad , \qquad \frac{dH}{dt} = 0$$

(we now know how to identify stencils that make Hamiltonians)

Assuming the decomposition

$$H = \underbrace{T(p)}_{\text{kinetic}} + \underbrace{V(q)}_{\text{potential}}$$

Then we want to solve

$$\dot{p} = -\partial_q V$$
$$\dot{q} = \partial_p T$$

Only works for separable Hamiltonian, no dissipation

Störmer - Verlet / Leapfrog integrator

$$\cancel{q_{n+1} = q_n + h\,\partial_p T(p_{n+1/2})}$$

$$p_{n+1/2} = q_n - \frac{h}{2}\partial_q V(q_n)$$
$$q_{n+1} = q_n + h\,\partial_p T(p_{n+1/2})$$
$$p_{n+1} = p_{n+1/2} - \frac{h}{2}\partial_q V(q_{n+1})$$