How to control $|R(z)|$?

$z = -Lh$

$\left.\begin{array}{l} ① \lim\limits_{z\to\infty} |R(z)| = 0. \\ ② \text{ A-stable.} \end{array}\right\}$ L- stable method.

Ex. Backward Euler.

$$R(z) = \frac{1}{1-z} \qquad \lim_{z\to\infty} |R(z)| = 0.$$

L- stable ✓ .

Ex. Trapezoidal.

$$R(z) = \frac{1+\frac{z}{2}}{1-\frac{z}{2}} \qquad \lim_{z\to\infty} |R(z)| = 1$$

L-stable ×.

Ex. GL1.

$$R(z) = \frac{1+\frac{z}{2}}{1-\frac{z}{2}}. \qquad \text{L-stable } \times.$$

Generalization.

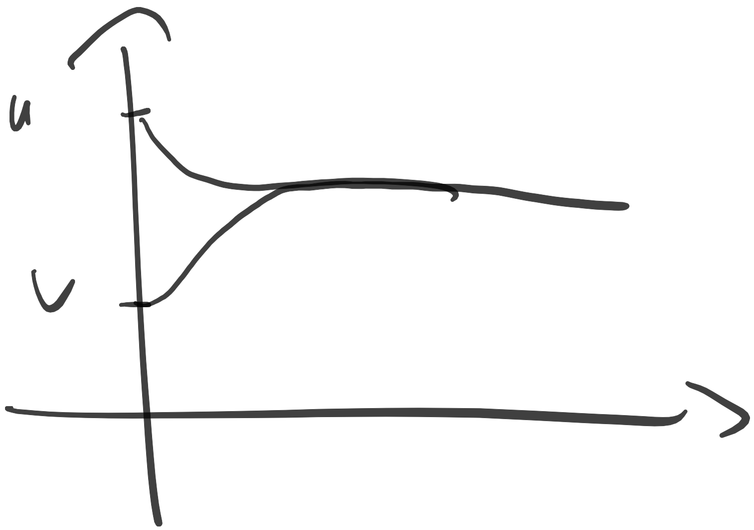
Contractive (a.k.a. dissipative) ODEs.

$$\begin{cases} \dot{u} = f(u,t), & u(0) = u_0 \\ \dot{v} = f(v,t), & v(0) = v_0. \end{cases}$$

$$E(t) = \| u(t) - v(t) \|_2^2$$

<u>Def</u>. ODE contractive if

$$\frac{dE(t)}{dt} \leq 0. \text{ for any } u(t), v(t)$$



$$\frac{dE}{dt} = 2\frac{d}{dt}\left[(u-v)^*(u-v)\right]$$

$$= 2\,\mathrm{Re}\,\left[f(u,t)-f(v,t)\right]^*(u-v)$$

$$= 2\,\mathrm{Re}\,\left(f(u,t)-f(v,t),\ u-v\right) \le 0.$$

Thm. ODE is contractive if

$$\mathrm{Re}\,(f(u,t) - f(v,t),\ u-v) \le 0.$$

$\forall\, u, v \in \mathbb{R}^d,\ t \in I.$

Ex. D-R example.

$$f(u,t) - f(v,t) = -L\,(u-v)$$

$$\mathrm{Re}\,(f(u,t) - f(v,t),\ u-v) = -L\,\|u-v\|_2^2 \le 0.$$

is contrative.

Requirement of numer. scheme.

<u>Def</u> A RK scheme is contractive.

(a.k.a. B-Stable) if for any numer. sol.

u_n, v_n of a contractive ODE

$$\|u_{n+1} - v_{n+1}\|_2 \le \|u_n - v_n\|_2 .$$

why B- stability?

$$u_{n+1} = u_n + h \sum_{i=1}^{r} b_i k_i(u_n)$$

$$u(t_{n+1}) = u(t_n) + h \sum_{i=1}^{r} b_i k(u(t_n)) + \tau_n$$

B- stable:

$$\| u(t_{n+1}) - u_{n+1} \| \le \| u(t_n) - u_n \| + \| \tau_n \|$$

$$\Rightarrow \| e_n \| \le \| \tau_0 \| + \cdots + \| \tau_{n-1} \| + \| e_0 \|$$

$T = hn.$

$$\le \frac{T}{h} \sup \| \tau \| + \| e_0 \|$$

no Lip const. involved.

Thm. B-stable $\Rightarrow$ A-stable.

Pf: $u' = \lambda u$, $\mathrm{Re}\,\lambda < 0$.

$$\mathrm{Re}\left(\lambda u - \lambda v,\ u - v\right) = \mathrm{Re}\,\lambda\ \|u - v\|^2 \leq 0$$

ODE is contractive.

$$\|u_{n+1} - v_{n+1}\| \leq \|u_n - v_n\| \quad \text{(B-stable)}$$

$$v_0 = 0 \Rightarrow v_n \equiv 0.$$

$\|u_{n+1}\| \leq \|u_n\| \leq \cdots \leq \|u_0\|$. no blow-up $\Rightarrow$ stable.

Ex. Backward Euler.

$$U_{n+1} = U_n + h\, f(U_{n+1}) \qquad , \; u \in \mathbb{R}^d.$$

$$V_{n+1} = V_n + h\, f(V_n)$$

$$\|U_{n+1} - V_{n+1}\|^2 = \Big(U_{n+1} - V_{n+1},\; U_n - V_n + h\big(f(U_{n+1}) - f(V_{n+1})\big) \Big)$$

$$\leq \left(U_{n+1} - V_{n+1},\; U_n - V_n \right)$$

$$\leq \|U_{n+1} - V_{n+1}\| \, \|U_n - V_n\|$$

$$\Rightarrow \|U_{n+1} - V_{n+1}\| \leq \|U_n - U_n\| \quad \Rightarrow \text{B-stable.}$$

(Exer) Trapezoidal is NOT B-stable.

Ex. GL1.

$$\begin{cases} k = f\left(u_n + \frac{h}{2}k\right) \\ u_{n+1} = u_n + hk \end{cases} \qquad u_n + \frac{h}{2}k = \frac{u_n + u_{n+1}}{2}$$

$$\|u_{n+1} - v_{n+1}\|^2 - \|u_n - v_n\|^2$$

use eq.

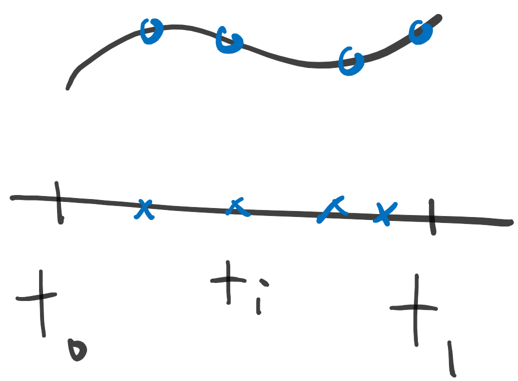
$$= (u_{n+1} - v_{n+1} + u_n - v_n,\ u_{n+1} - v_{n+1} - u_n + v_n)$$

$$= 2h\left(\frac{u_{n+1}+u_n}{2} - \frac{v_{n+1}+v_n}{2},\ f\left(\frac{u_{n+1}+u_n}{2}\right) - f\left(\frac{v_{n+1}+v_n}{2}\right)\right) \le 0.$$

$\Rightarrow$ GL1 B stable.

Thm. GL methods are B-stable.

Pf.



$t_i = t_0 + c_i h$, $i = 1, \cdots, r$.

$b_i = \int_0^1 \tilde{P}_i(\theta)\, d\theta \geq 0$.

$u_1 = u_0 + h \sum_{i=1}^{r} b_i k_i$.

$u_1 = \tilde{u}(t_1)$, $u_i = \tilde{u}(t_i)$

$k_i = f(\tilde{u}(t_i))$

$\tilde{u}(t) \in \mathbb{P}_r$,

so is $\tilde{v}(t)$

$E(t) = \| \tilde{u}(t) - \tilde{v}(t) \|^2$

want to show $E(t_1) \le E(t_0)$

only satisfied at $t = t_i$

$E'(t) = 2 \left(\tilde{u}(t) - \tilde{v}(t), f(\tilde{u}(t)) - f(\tilde{v}(t)) \right) \le 0$.

$E(t_1) = E(t_0) + \int_{t_0}^{t_1} E'(s)\, ds$

only know pts evaluated at t_i

poly. order $2r-1$

Gauss quad. is exact.

$= E(t_0) + h \sum_{i=1}^{r} b_i E'(t_i)$

$\le E(t_0)$

$\Longrightarrow$ GL. B-stable.

Hamiltonian system.

Newtonian dynamics.

particle at position $q(t)$

momentum $p(t) = m\dot{q}(t)$

force given by potential field $V(q)$

$$f(q(t)) = -D_q V(q(t))$$

$$\dot{p}(t) = -D_q V(q(t)) \quad \leftarrow \text{ Newton's law.}$$

$$\begin{cases} \dot{p} = -D_q V(q) \\ \dot{q} = \dfrac{p}{m} \end{cases}$$

Hamiltonian (a.k.a. energy)

$$H(p, q) = \frac{p^2}{2m} + V(q)$$

Preserved along dynamics

$$\frac{d}{dt} H\big(p(t), q(t)\big) = \frac{p \cdot \dot{p}}{m} + D_q V(q)\, \dot{q}$$

$$= \frac{p}{m} \cdot \left(-D_q V(q)\right) + D_q V(q) \cdot \frac{p}{m} = 0 .$$

$$H(p(t), q(t)) = H(p(0), q(0)) \leftarrow \text{initial energy}$$

Hamiltonian : $H : \underset{\substack{\uparrow \\ \text{momentum}}}{\mathbb{R}^d} \times \underset{\substack{\uparrow \\ \text{position}}}{\mathbb{R}^d} \longrightarrow \mathbb{R}$.

$$\begin{cases} \dot{p}(t) = -\dfrac{\partial H}{\partial q}(p(t), q(t)) \\ \dot{q}(t) = \dfrac{\partial H}{\partial p}(p(t), q(t)) \end{cases}$$ Hamiltonian dyn.

Ex. $H(p, q) = \dfrac{p^2}{2m} + V(q)$.

$$\frac{\partial H}{\partial p} = \frac{p}{m}$$

$$\frac{\partial H}{\partial q} = D_q V(q).$$

Separable Ham. system.

$$H(p,q) = T(p) + V(q)$$

Ex. N particles $(p_1, \dots, p_N)$ momentum

$(q_1, \dots, q_N)$ position.

$$T(p) = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} \quad . \quad V(q)$$

$$\begin{cases} \dot{p}_i = -\nabla_{q_i} V(q_1, \dots, q_N) \\ \dot{q}_i = \dfrac{p_i}{m_i} \end{cases}$$

Whether numer. scheme would produce a dynamics that conserves energy (more generally. constraints)

Geometric integrator.

[Hairer. Lubich. Wanner. 2006]

Most schemes cannot satisfy constraints.

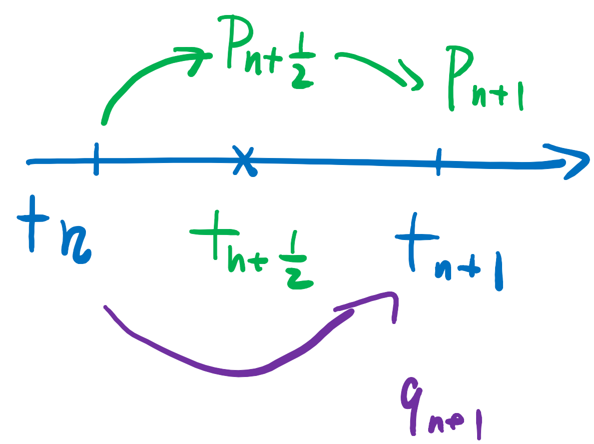
Long time evolution.

Ex. good scheme. Strömer-Verlet.

$$T(p) = \frac{p^2}{2m}, \quad V(q)$$

$$(p_n, q_n) \longrightarrow (p_{n+1}, q_{n+1})$$

$$\begin{cases} p_{n+\frac{1}{2}} = p_n - \frac{h}{2} D_q V(q_n) \\ q_{n+1} = q_n + h\, p_{n+\frac{1}{2}} \\ p_{n+1} = p_{n+\frac{1}{2}} - \frac{h}{2} D_q V(q_{n+1}) \end{cases}$$



2nd order explicit method.

Ex. Harmonic oscillator

$$\ddot{q} = -q. \qquad H(p,q) = \frac{1}{2}p^2 + \frac{1}{2}q^2$$

Ex. $\ddot{q} = -\sin q. \qquad H(p,q) = \frac{1}{2}p^2 - \cos q.$

$u = (p, q)^T$

$t = 0. \quad \Omega = \{ u \in \mathbb{R}^2 \mid (u_1 - 3)^2 + u_2^2 \le 0.3^2 \}.$

flow map. $\varphi_t(u_0) = u(t)$

$$\varphi_t(\Omega)$$

In $\mathbb{R}^2$. area preservation. $\Rightarrow$ Jacobian. has determinant 1.

$$u(t) = \varphi_t(u_0)$$

$$\Phi_t = \begin{bmatrix} \frac{\partial p(t)}{\partial p_0} & \frac{\partial p(t)}{\partial q_0} \\ \frac{\partial q(t)}{\partial p_0} & \frac{\partial q(t)}{\partial q_0} \end{bmatrix}.$$

$$|\Phi_t| \equiv 1$$

want to show.

<u>Def</u>. $J = \begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix} \in \mathbb{R}^{2d \times 2d}$.

$$\frac{du}{dt} = \begin{pmatrix} \frac{dp}{dt} \\ \frac{dq}{dt} \end{pmatrix} = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial p} \\ \frac{\partial H}{\partial q} \end{bmatrix} = J^{-1} D_u H(u)$$

$$\left(J^{-1} = -J = J^{T} \right)$$

$$\frac{d}{dt} \Phi_t = \frac{d}{dt} \frac{\partial \varphi_t}{\partial u_0} = \frac{\partial}{\partial u_0} \left(J^{-1} \nabla_u H(\varphi_t(u_0)) \right)$$

$$= J^{-1} \nabla^2 H(\varphi_t(u_0)) \Phi_t$$

$$\frac{d}{dt} \left(\Phi_t^T J \Phi_t \right) = \left(\frac{d}{dt} \Phi_t \right)^T J \Phi_t + \Phi_t^T J \left(\frac{d}{dt} \Phi_t \right)$$

$$= \Phi_t^T \nabla^2 H (-J^{-1}) J \Phi_t + \Phi_t^T J J^{-1} \nabla^2 H \Phi_t = 0 .$$

$$\Rightarrow \Phi_t^T J \Phi_t = \Phi_0^T J \Phi_0 = J .$$

$$\Phi_0 = \frac{\partial \varphi_0(u_0)}{\partial u_0} = I_{2d}$$

Def. $\varphi : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d \times \mathbb{R}^d$ flow map is symplectic if $\Phi(u) := \frac{\partial \varphi(u)}{\partial u}$ satisfies

$$\Phi^T(u)\, J\, \Phi(u) = J.$$

Thm. (Poincaré) Hamiltonian dyn.

$\varphi_t(u_0)$ is symplectic for any $t \geq 0$.

Pf: above.

In $\mathbb{R}^2$.

$$\Phi_t^T J \Phi_t = \begin{bmatrix} \frac{\partial p}{\partial p_0} & \frac{\partial q}{\partial p_0} \\ \frac{\partial p}{\partial q_0} & \frac{\partial q}{\partial q_0} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial p}{\partial p_0} & \frac{\partial p}{\partial q_0} \\ \frac{\partial q}{\partial p_0} & \frac{\partial q}{\partial q_0} \end{bmatrix}$$

$$= \left(\frac{\partial p}{\partial p_0} \frac{\partial q}{\partial q_0} - \frac{\partial p}{\partial q_0} \frac{\partial q}{\partial p_0} \right) \cdot \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$= |\Phi_t| \, J$$

By Poincaré thm. $\Phi_t^T J \Phi_t = J$

$\Rightarrow |\Phi_t| \equiv 1$ for all t. $\Rightarrow$ area preservation!

Def. Nume. scheme. generates a discrete flow map $\varphi_n : u_0 \mapsto u_n$. is symplectic if for each n, φ_n is a symplectic map.

One step method.

$$u_{n+1} = \Phi(u_n)$$

Φ is symplectic $\Longleftrightarrow$ φ_n is symplectic for all n.

Pf: Only need to show $\Rightarrow$.

$$\frac{\partial \varphi_{n+1}}{\partial u_0} = \frac{\partial \Psi}{\partial u}(u_n)\,\frac{\partial \varphi_n}{\partial u_0}$$

$$\left(\frac{\partial \varphi_{n+1}}{\partial u_0}\right)^T J \left(\frac{\partial \varphi_{n+1}}{\partial u_0}\right) = \left(\frac{\partial \varphi_n}{\partial u_0}\right)^T \underbrace{\left[\frac{\partial \Psi}{\partial u}(u_n)^T J\, \frac{\partial \Psi}{\partial u}(u_n)\right]}_{J.\ \text{since } \Psi \text{ is symplectic}} \left(\frac{\partial \varphi_n}{\partial u_0}\right)$$

$$= \left(\frac{\partial \varphi_n}{\partial u_0}\right)^T J \left(\frac{\partial \varphi_n}{\partial u_0}\right)$$

Proof by induction.