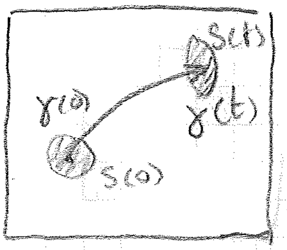
Symplectic dynamics

recall dynamical system:

$\begin{cases} \text{phase space } \Gamma\text{, coordinate } \gamma \\ \text{eqs of motion } \dot\gamma = f(\gamma, t) \end{cases}$

γ in our case $= r_1, r_2 \dots r_N\ v_1, v_2 \dots v_N$

Numerical & integration errors mean you are never exactly in the right spot. So let's look at the neighbourhood.



Γ small volume $S(0)$ around $\gamma(0)$

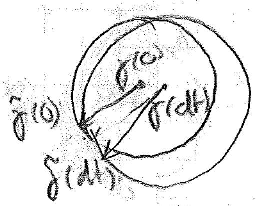
$\gamma(0) \to \gamma(t) \quad : \quad S(0) \to S(t)$

$\dot S(t)$?

$\gamma(dt) = \gamma(0) + dt \left.\frac{\partial\gamma}{\partial t}\right|_{\gamma=\gamma_0}$ tho.

$\quad = \gamma(0) + dt\, f(\gamma(0))$

$\tilde\gamma(dt) = \tilde\gamma(0) + dt\, f(\tilde\gamma(0))$



$\gamma(t) + \delta\gamma(t) = \tilde\gamma(t)$

$\delta\gamma(dt) = \tilde\gamma(dt) - \gamma(dt)$

$= \tilde\gamma(0) + dt\, f(\tilde\gamma(0)) - \gamma(0) - dt\, f(\gamma(0))$

$= \delta\gamma(0) + dt\left[f(\tilde\gamma(0)) - f(\gamma(0))\right]$ Taylor in $\gamma(0)$

$= \delta\gamma(0) + dt \left.\frac{\partial f}{\partial\gamma}\right|_{\gamma=\gamma(0)} \cdot \delta\gamma(0) = \underbrace{\left(\mathbb{1} + dt \left.\frac{\partial f}{\partial\gamma}\right|_{\gamma=\gamma_0}\right)}_{M} \cdot \delta\gamma(0)$

$M \leftarrow$ Jacobian

volume spanned by $\delta\gamma$ vectors is multiplied by $\det M \qquad S(t) = S(0) \det M$ tho.

eigenvalues of $\left.\frac{\partial f}{\partial\gamma}\right|_{\gamma=\gamma(0)}$ are $\lambda_1, \lambda_2, \dots$

$\frac{d}{dt}\ln S = \frac{1}{dt}\left[\ln S(dt) - \ln S(0)\right] = \frac{1}{dt}\ln\det M$

$= \frac{1}{dt}\ln\prod_i (1 + dt\,\lambda_i) = \frac{1}{dt}\sum_i dt\,\lambda_i = \mathrm{Tr}\left.\frac{\partial f}{\partial\gamma}\right|_{\gamma=\gamma(0)}$

Hamiltonian dynamical systems (conserved E)

$\dot p = -\frac{\partial H}{\partial q} \quad \dot q = \frac{\partial H}{\partial p} \qquad \gamma = (p, q) \quad f(\gamma) = \left(-\frac{\partial H}{\partial q}, \frac{\partial H}{\partial p}\right)$

$\frac{\dot S(t)}{S} = \frac{\partial}{\partial\gamma}\cdot f(\gamma, t) = \frac{\partial}{\partial p}\cdot\left(-\frac{\partial H}{\partial q}\right) + \frac{\partial}{\partial q}\cdot\frac{\partial H}{\partial p} = 0$

explain a bit more

conserving phase space volume = symplectic

- if contraction: areas the system eventually will no longer visit.
- time reversal symmetry.

Verlet integration and phase space volume

$$r(t+h) = r(t) + h\,v(t) + h^2 a(t)/2$$
$$v(t+h) = v(t) + h[a(t+h) + a(t)]/2$$
velocity verlet

Volume change: Jacobian

$$\det \begin{pmatrix} \frac{\partial r(t+h)}{\partial r(t)} & \frac{\partial v(t+h)}{\partial r(t)} \\ \frac{\partial r(r+h)}{\partial v(t)} & \frac{\partial v(t+h)}{\partial v} \end{pmatrix} =$$

$$\text{''} \; 1 + \tfrac{1}{2}h^2 \frac{\partial a}{\partial r}$$

$$\det \begin{pmatrix} 1 + \frac{1}{2}h^2 \frac{\partial a}{\partial r} & \frac{1}{2}h\left[\frac{\partial a}{\partial r} \frac{\partial r(t+h)}{\partial r} + \frac{\partial a}{\partial r}(t)\right] \\ h & 1 + \frac{1}{2}h \frac{\partial a}{\partial r} h \end{pmatrix}$$

$$= 1 + h^2 \frac{\partial a}{\partial r} + \frac{1}{4}\cancel{h^4\left(\frac{\partial a}{\partial r}\right)^2} - \frac{1}{2}h^2 \frac{\partial a}{\partial r}\left[\left(1 + \cancel{\tfrac{1}{2}h^2 \frac{\partial a}{\partial r}}\right) + 1\right]$$

$= 1 +$ everything cancels

$\Rightarrow$ conserves phase space volume exactly,
dynamics really act Hamiltonian

$\Rightarrow$ There is another, similar Hamiltonian $\hat{H}$, whic describes the calculated trajectory exactly

$\Rightarrow$ Error in E is bounded $\Rightarrow$ no silly blowups

---

Overview algorithms.

	Verlet	RK 4
	- less work / time step - error $O(h^4)$ - only Hamiltonian systems or simple modifications of those - symplectic $\Rightarrow$ robust	- error $O(h^5)$, so time step can be larger $\Rightarrow$ fewer time steps - any eqs. of motion - suitable for variable time step (RK-Fehlberg)
use if	E conserved or viscous damping	otherwise

There are other options as well