Example (1) Mathematical Pendulum

$'$ = derivative
$''$ = second derivative

$x(t)$: angle $\leftrightarrow q$

$x'(t)$: angular velocity $\leftrightarrow p$ "momentum"

$$\begin{cases} x'' + \sin(x) = 0 \\ x(0)=1,\ x'(0)=0 \end{cases} \Leftrightarrow \begin{cases} x' = y, & x(0)=1 \\ y' = -\sin(x), & y(0)=0 \end{cases} \quad (*)$$

Hamiltonian, "total energy": $\mathcal{H}(x,y) = \frac{1}{2}y^2 + (1-\cos(x)) = \text{constant (in time)}$

($\frac{1}{2}y^2$: kinetic energy; $1-\cos(x)$: potential energy)

$$\frac{\partial \mathcal{H}}{\partial x} = \sin(x), \quad \frac{\partial \mathcal{H}}{\partial y} = y \Rightarrow \begin{cases} x' = \frac{\partial \mathcal{H}}{\partial y} \\ y' = -\frac{\partial \mathcal{H}}{\partial x} \end{cases}$$ check (*)

$$\Leftrightarrow \begin{pmatrix} x \\ y \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial \mathcal{H}}{\partial x} \\ \frac{\partial \mathcal{H}}{\partial y} \end{pmatrix}$$

skew-symmetric matrix A

symmetric matrix: $A = A^T$ ← "transpose" (switch elements of matrix via the diagonal)

skew-symmetric: $A = -A^T$

here: $A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, $A^T = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, $-A^T = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

$$\frac{d\mathcal{H}}{dt} = \frac{d}{dt}\mathcal{H}(x,y) = \frac{\partial \mathcal{H}}{\partial x}\cdot\frac{dx}{dt} + \frac{\partial \mathcal{H}}{\partial y}\cdot\frac{dy}{dt} = \frac{\partial \mathcal{H}}{\partial x}x' + \frac{\partial \mathcal{H}}{\partial y}y' =$$

(↑ chain rule; ↑ our notation)

$$= \sin(x)\cdot y + y\cdot -\sin(x) = 0$$

$\Rightarrow \mathcal{H}$ is constant in time

Example ② predator-prey model ("Volterra-Lotka")

$$\begin{cases} x' = x - xy \\ y' = xy - y \end{cases}$$

$x(t)$: prey
$y(t)$: predator

$' = \frac{d}{dt}$

"energy" $\mathcal{H} = x - \ln(x) + y - \ln(y) = \text{constant (in time)}$

$$\frac{\partial \mathcal{H}}{\partial x} = 1 - \frac{1}{x} = \frac{x-1}{x}, \quad \frac{\partial \mathcal{H}}{\partial y} = 1 - \frac{1}{y} = \frac{y-1}{y}$$

$$\begin{pmatrix} x \\ y \end{pmatrix}' = \begin{pmatrix} 0 & -xy \\ xy & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial \mathcal{H}}{\partial x} \\ \frac{\partial \mathcal{H}}{\partial y} \end{pmatrix}$$

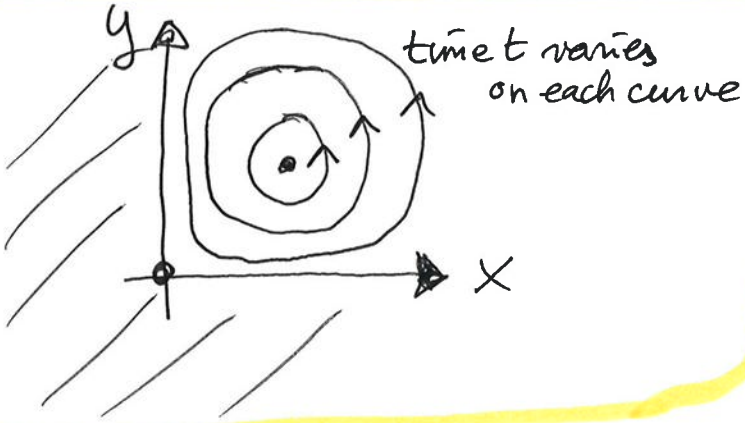
skew-symmetric matrix

$$\Rightarrow \frac{d\mathcal{H}}{dt} = \frac{\partial \mathcal{H}}{\partial x} x' + \frac{\partial \mathcal{H}}{\partial y} y' = \frac{\partial \mathcal{H}}{\partial x} \cdot (x - xy) + \frac{\partial \mathcal{H}}{\partial y} \cdot (xy - y)$$

$$= \frac{x-1}{x} \cdot (x - xy) + \frac{y-1}{y} \cdot (xy - y)$$

$$= (x-1) \cdot (1-y) + (y-1) \cdot (x-1) = 0$$

$\Rightarrow \mathcal{H}$ is constant in time.



Example ③ Hénon-Heiles model

(stellar dynamics, also in chemical reaction paths)
"two coupled non-linear oscillators"

Hamiltonian $\mathcal{H}(x, y, P_x, P_y) = \frac{1}{2}(P_x^2 + P_y^2) + \frac{1}{2}(x^2 + y^2) + \lambda\left(x^2 y - \frac{1}{3}y^3\right)$

4 variables: $x(t), y(t), P_x(t), P_y(t)$; λ parameter

$$x' = \frac{\partial \mathcal{H}}{\partial P_x},\quad y' = \frac{\partial \mathcal{H}}{\partial P_y},\quad P_x' = -\frac{\partial \mathcal{H}}{\partial x},\quad P_y' = -\frac{\partial \mathcal{H}}{\partial y}$$

$' = \frac{d}{dt}$

define: $\vec{q} = \begin{pmatrix} x \\ y \end{pmatrix}$ and $\vec{p} = \begin{pmatrix} P_x \\ P_y \end{pmatrix}$, then $\mathcal{H} = \mathcal{H}(\vec{q}, \vec{p})$

$$\begin{pmatrix} x \\ y \\ P_x \\ P_y \end{pmatrix}' = \underbrace{\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}}_{\text{skew-symmetric}} \begin{pmatrix} \partial\mathcal{H}/\partial x \\ \partial\mathcal{H}/\partial y \\ \partial\mathcal{H}/\partial P_x \\ \partial\mathcal{H}/\partial P_y \end{pmatrix}$$

$$\Leftrightarrow \begin{cases} x' = P_x \\ y' = P_y \\ P_x' = -x - \lambda x y \\ P_y' = -y - \lambda x^2 + \lambda y^2 \end{cases}$$

(four differential equations)

$$\frac{d\mathcal{H}}{dt} = \frac{\partial \mathcal{H}}{\partial x} x' + \frac{\partial \mathcal{H}}{\partial y} y' + \frac{\partial \mathcal{H}}{\partial P_x} P_x' + \frac{\partial \mathcal{H}}{\partial P_y} P_y'$$

$$= \text{---} = 0$$

$\mathcal{H}$ is constant (in time)

Example 4 — The three-dimensional Lorenz system

$' = \frac{d}{dt}$ ✳

$$\begin{cases} x' = \sigma(y-x) \\ y' = r\,x - y - xz \\ z' = xy - bz \end{cases}$$

$\sigma, r, b > 0$ — σ: Prandtl number; r: Rayleigh number; b: geometric aspect ratio

$\Leftrightarrow \vec{X}' = \vec{f}(\vec{X})$ with $\vec{X} = (x,y,z)^T$ and $\vec{f} = (\underbrace{\sigma(y-z)}_{f_1}, \underbrace{rx-y-xz}_{f_2}, \underbrace{xy-bz}_{f_3})^T$

calculate:

$$\nabla \cdot \vec{f} = \frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} + \frac{\partial f_3}{\partial z} = -(\underbrace{\sigma + 1 + b}_{>0}) < 0$$

$\Rightarrow$ system is <u>dissipative</u>, the trajectories/solutions/curves $x(t), y(t), z(t)$ are "forced onto a zero-volume attractor where chaotic dynamics occur"!

the undamped/conservative Lorenz system

$$\begin{cases} x' = \sigma y \\ y' = -xz \\ z' = xy \end{cases}$$ ✳

$$\Rightarrow \nabla \cdot \vec{f} = \frac{\partial}{\partial x}(\sigma y) + \frac{\partial}{\partial y}(-xz) + \frac{\partial}{\partial z}(xy) = 0$$

"phase-space volume is strictly conserved"

$\Rightarrow$ <u>no</u> attractors (no strange attractors)

(no chaotic behaviour.

$\mathcal{H}_1(x,y,z) = y^2 + z^2 = C_1$ (constant)

$\mathcal{H}_2(x,y,z) = x^2 - 2\sigma z = C_2$ (other constant)

check ... $\frac{d\mathcal{H}_1}{dt} = \frac{\partial \mathcal{H}_1}{\partial x}x' + \frac{\partial \mathcal{H}_1}{\partial y}y' + \frac{\partial \mathcal{H}_1}{\partial z}z' = \dots = 0$

also: $\frac{d\mathcal{H}_2}{dt} = \dots = 0$ (!)

✳ can be re-written

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}' = \underbrace{\begin{pmatrix} 0 & \sigma & 0 \\ -\sigma & 0 & -x \\ 0 & x & 0 \end{pmatrix}}_{\text{skew-symmetric matrix}} \begin{pmatrix} \partial\mathcal{H}_1/\partial x \\ \partial\mathcal{H}_1/\partial y \\ \partial\mathcal{H}_1/\partial z \end{pmatrix}$$

Other examples

Lennard-Jones potential

two molecules: $r = \|\vec{r}\| = \sqrt{x^2+y^2+z^2}$ distance between the two molecules

ε = depth of potential well ("Bond energy")

σ = distance to where $V(r) = 0$

Hamiltonian $\mathcal{H}(\vec{r}, \vec{p})$

$$= \frac{\|\vec{p}\|^2}{2m} + V(r) = \frac{p_x^2+p_y^2+p_z^2}{2m} + 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$\begin{cases} x' = \frac{\partial \mathcal{H}}{\partial p_x} = \frac{p_x}{m}, \; y' = \frac{\partial \mathcal{H}}{\partial p_y} = \frac{p_y}{m}, \; z' = \frac{\partial \mathcal{H}}{\partial p_z} = \frac{p_z}{m} \\ \text{force } \vec{F} = -\nabla V(r) \\ \vec{p}' = \frac{24\varepsilon}{r^2}\left[2\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \\ \text{six differential equations} \end{cases}$$

$$\Rightarrow \frac{d\mathcal{H}}{dt} = \nabla_{\vec{r}}\mathcal{H} \cdot \vec{r}' + \nabla_{\vec{p}}\mathcal{H} \cdot \vec{p}' = \cdots = 0$$

$\mathcal{H}$ is constant (in time)

restricted two-body system

$M \gg m$ (earth (mass m) $\leftrightarrow$ sun (mass M) for example)

$$\mathcal{H}(x, y, p_x, p_y) = \frac{p_x^2+p_y^2}{2m} - \frac{k}{\sqrt{x^2+y^2}}$$

; $r = \sqrt{x^2+y^2}$ distance to the "origin"

$k = GMm$ (gravitational potential)

$$\begin{cases} x' = \frac{\partial \mathcal{H}}{\partial p_x} = \frac{p_x}{m}, \; y' = \frac{\partial \mathcal{H}}{\partial p_y} = \frac{p_y}{m} \\ p_x' = -\frac{\partial \mathcal{H}}{\partial x} = \frac{-kx}{(x^2+y^2)^{3/2}}, \; p_y' = -\frac{\partial \mathcal{H}}{\partial y} = \frac{-ky}{(x^2+y^2)^{3/2}} \\ \text{four differential equations} \end{cases}$$

$$\Rightarrow \frac{d\mathcal{H}}{dt} = \frac{\partial \mathcal{H}}{\partial x}x' + \frac{\partial \mathcal{H}}{\partial y}y' + \frac{\partial \mathcal{H}}{\partial p_x}p_x' + \frac{\partial \mathcal{H}}{\partial p_y}p_y' = \cdots = 0$$

$\mathcal{H}$ is constant (in time).

How do we find solutions for differential equations in general, and for Hamiltonian systems with energy $\mathcal{H}$ in particular?

First, consider the partial differential equation:

(PDE)

$$\frac{\partial u}{\partial t} = \varepsilon \cdot \Delta u + D \cdot (1 + a - u)\, e^{-\delta/u}$$

- $\frac{\partial u}{\partial t}$: (partial) time-derivative
- ε: diffusion coefficient
- Δu: div(grad(u))
- $D \cdot (1 + a - u)\, e^{-\delta/u}$: reaction term

$$D = \frac{Re^{\delta}}{a\delta}$$

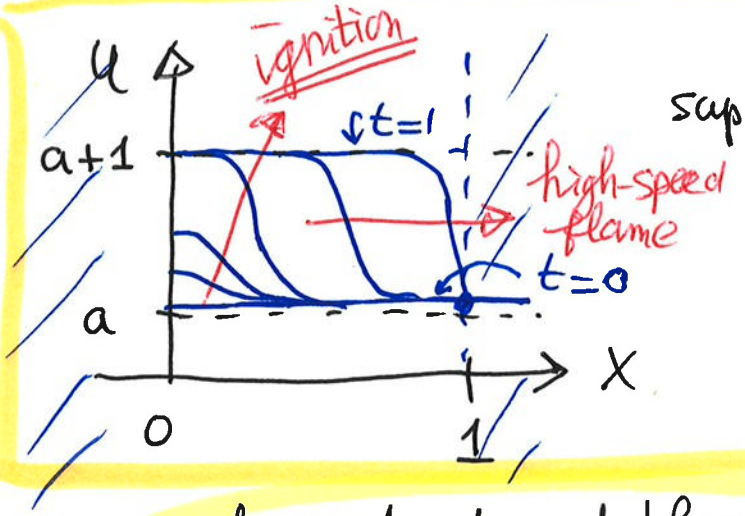
- D: Damkohler number
- R: reaction rate
- a: heat exchange
- δ: activation energy

This is a (PDE) model for the temperature $u(x,y,z,t)$ of a reactant in a chemical system.

In one space dimension ("1D"): $u(x,t)$ and $\Delta u = \frac{\partial^2 u}{\partial x^2}$

solutions ???

how ?



suppose $u(x,0) = a$ for $x \in (0,1)$

$\uparrow$ $t=0$

how do I get these graphs ?

one step simpler: $\varepsilon = 0$ $\Rightarrow$ ordinary differential equation

take $a=1$ and $u(0)=1$:

$$\begin{cases} u'(t) = D\cdot(2-u(t))\,e^{-\delta/u(t)} \\ u(0) = 1 \end{cases}$$

$u(t) = ?$

D, δ known

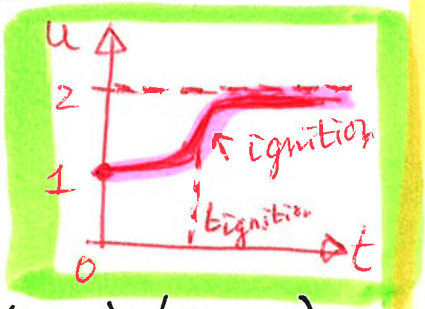
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separation of variables ?

check: $\dfrac{du}{dt} = D(2-u)e^{-\delta/u} \Leftrightarrow \dfrac{du}{D(2-u)e^{-\delta/u}} = dt$

$$\Leftrightarrow \int \frac{du}{D(2-u)e^{-\delta/u}} = \int dt$$

$= ???$ $\qquad = t + C$



no primitive (or anti-derivative is known)

$\not\Rightarrow$ $u(t) = \text{---}$???

we need to find numerical solutions (with the computer)

We start with a (slightly) more general situation

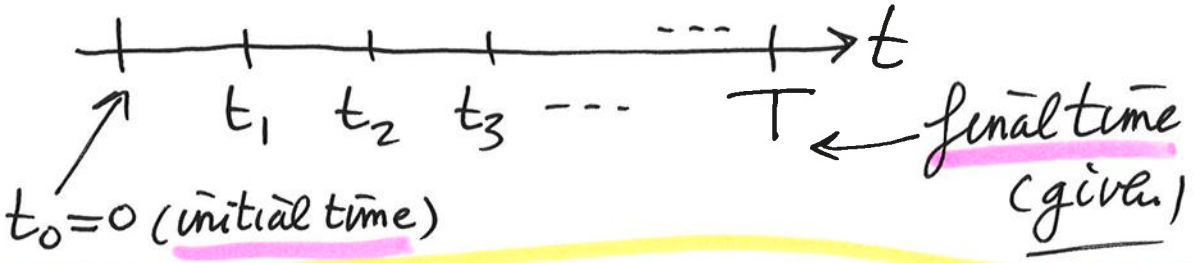
Consider $\begin{cases} u'(t) = f(u(t), t) \\ u(t_0) = u_0 \end{cases}$

f: given function, for example: $\cos(t) \cdot (u(t))^2$

u_0: given value

t_0: mostly $= 0$

1) divide the t-axis ("time t") in a finite number of equal intervals.



2) call every sub-interval: Δt (or h)

then: $t_0 = 0 = 0 \cdot \Delta t$

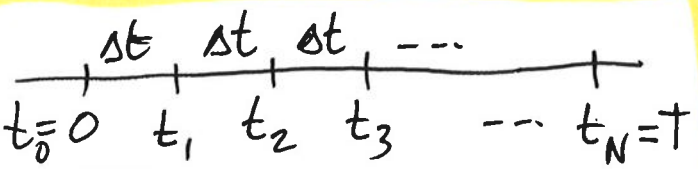
$t_1 = t_0 + \Delta t = 1 \cdot \Delta t$

$t_2 = t_1 + \Delta t = 2 \cdot \Delta t$

$\vdots$

$t_N = t_{N-1} + \Delta t = T = N \cdot \Delta t$

N = the number of steps to arrive at $t = T$



3) call the exact (but unknown!) values of the solution in the time points $t_0, t_1, \dots, t_N$:

$$u(t_0), u(t_1), u(t_2), \dots, u(t_N)$$

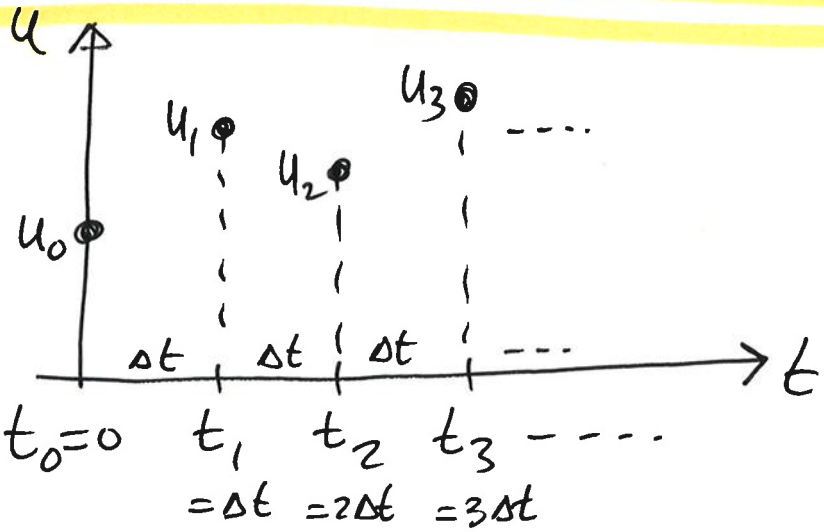
(goal: we would like to approximate these values, a finite number of values (!) as good as possible)

4) call the approximations via the computer (yet to be determined!): $u_0, u_1, u_2, \dots, u_N$ (at $t_0, t_1, \dots, t_N$)

so: $u(t_0) \approx u_0, u(t_1) \approx u_1, \dots, u(t_N) \approx u_N$

↑ note that u_0 is given $\Rightarrow u(t_0) = u_0$ ↑

in a diagram:



- how do we find $u_1, u_2, \dots$?
- how good is the approximation?
- does this depend on Δt (or N)?
- what happens for "$\Delta t \to 0$" ("convergence to exact solution")?
- are there other issues to be checked ... ? (YES, see later)

Examine "the" definition of derivative:

$$u'(t) = \lim_{\Delta t \to 0} \frac{u(t+\Delta t) - u(t)}{\Delta t}$$

or ... $\lim_{\Delta t \to 0} \frac{u(t) - u(t-\Delta t)}{\Delta t}$ ... or ... $\lim_{\Delta t \to 0} \frac{u(t+\Delta t) - u(t-\Delta t)}{2\Delta t}$ or ... ?!

for "small" Δt: $u'(t) \approx \frac{u(t+\Delta t) - u(t)}{\Delta t}$

the DE says: $u(t)$ must satisfy $u'(t) = f(u(t), t)$ at each time point t

$$\Longrightarrow \frac{u(t+\Delta t) - \Delta t}{\Delta t} \approx f(u(t), t)$$

"Taylor" (!)

$$\left[\Leftrightarrow u(t+\Delta t) \approx u(t) + \Delta t \cdot u'(t) = u(t) + \Delta t \cdot f(u(t), t) \right]$$

f is given, Δt is chosen

Suppose we have the value $u(t)$ at time t

then we can calculate $u(t+\Delta t)$ at the next time point $t+\Delta t$.

$t+\Delta t$ to $t+2\Delta t$

$$\Longrightarrow u(t+2\Delta t) \approx u(t+\Delta t) + \Delta t \cdot f(u(t+\Delta t), t+\Delta t)$$

chosen; given; known; just calculated from $u(t)$!

then also possible:

$$u(t+3\Delta t) \approx u(t+2\Delta t) + \Delta t \cdot f(u(t+2\Delta t), t+2\Delta t)$$

chosen, given, known, just calculated from $u(t+\Delta t)$

etcetera ... !

sequence:
- $u(t+\Delta t)$ ...
- $u(t+2\Delta t)$ ---▸
- $u(t+3\Delta t)$:
- ------
- etcetera

$\Longrightarrow$

$$u_1 = u_0 + \Delta t\, f(u_0, t_0)$$
$$u_2 = u_1 + \Delta t\, f(u_1, t_1)$$
$$u_3 = u_2 + \Delta t\, f(u_2, t_2)$$
$$\vdots \qquad \vdots \qquad \vdots$$
$$u_N = u_{N-1} + \Delta t\, f(u_{N-1}, t_{N-1})$$

The "recipe" becomes:

at $t=0$ { u_0 given, $t_0 = 0$

$$\left.\begin{aligned} u_{n+1} &= u_n + \Delta t\, f(u_n, t_n) \\ t_{n+1} &= t_n + \Delta t \end{aligned}\right\} \; n = 0, 1, 2, \dots, N-1$$

gives $u_N = \dots$

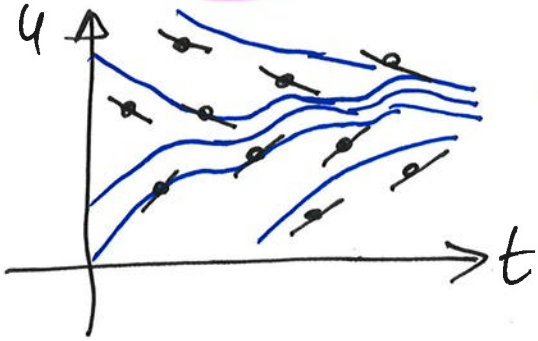
This method/algorithm is called Euler-Forward or Explicit Euler

↑ "EF"

It is an explicit numerical method: one can calculate the numerical values (approximations) directly from the previously calculated numerical values.

A graphical interpretation of EF:

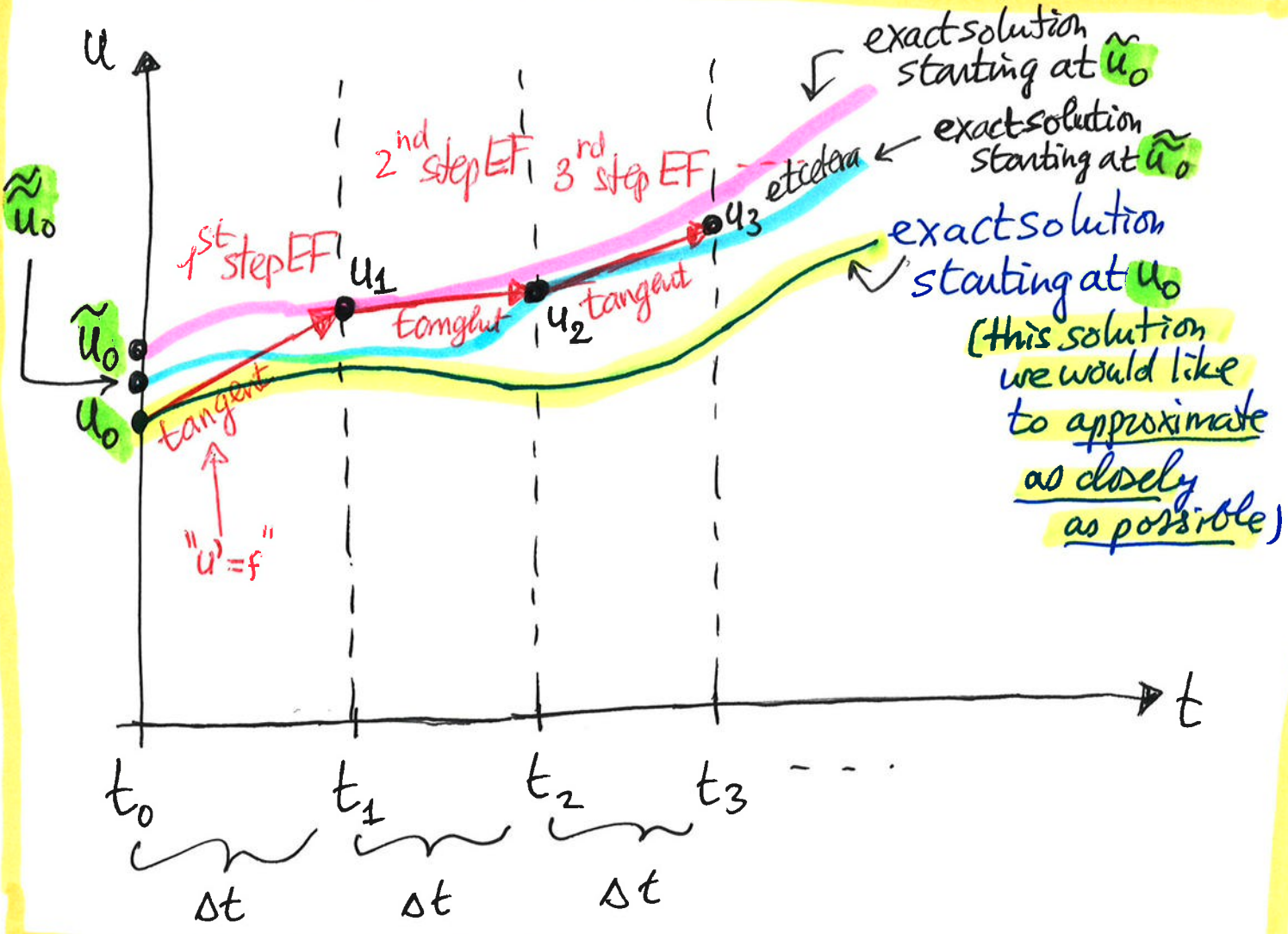
remember the direction field of an ordinary DE



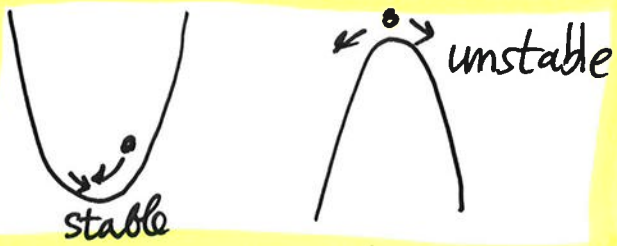
exact solutions follow the direction field

"the $\nearrow$" in the figure

for each (t,u) we know u', since $u' = f$ ← given



- How accurate is this approximation?
- What could happen, if the initial value u_0 is slightly perturbed (for example, by rounding errors)?
  ↳ "numerical stability"



- Other methods?
- For Hamiltonian DEs?

numerical solution: $u_{n+1} = u_n + \Delta t \cdot f(u_n, t_n)$ ⊙

Taylor about time point t_n:

$$u(t_{n+1}) = u(t_n) + (t_{n+1} - t_n) \cdot u'(t_n) + \frac{(t_{n+1} - t_n)^2}{2} \cdot u''(t_n) + \dots$$

$$\approx u(t_n) + \Delta t \cdot f(u(t_n), t_n) + \frac{(\Delta t)^2}{2} u''(t_n)$$

on the interval (t_n, t_{n+1}): the difference between the approximation formula ⊙ and the (almost) exact Taylor formula

$$\approx \frac{1}{2} (\Delta t)^2 u''(t_n)$$

step size squared; 2nd derivative of the (unknown) solution at $t = t_n$

This is a local error on the interval (t_n, t_{n+1}).

→ u'' can vary a lot (depends on the DE)

→ it suggests that the error in the approximation decreases quadratically with Δt decreasing.

However, this local error is made on each interval

$(t_0,t_1),(t_1,t_2),(t_2,t_3),\dots\dots,(t_{n-1},t_n)$

n – intervals, each with an error $\approx (\Delta t)^2$

$\Rightarrow$ "the" error at $t=t_n \approx n.(\Delta t)^2 \approx (\Delta t)^1$

global error is approximately constant. Δt.

(linear decrease)

* numerical stability

check the "test" model: $\begin{cases} u' = \lambda u \\ u(0) = u_0 \end{cases}$, $\lambda < 0$

and the "perturbed" model: $\begin{cases} \tilde{u}' = \lambda \tilde{u} \\ \tilde{u}(0) = u_0 + \varepsilon \end{cases}$ ↑ "small"

Apply EF to both DE-models:

$\begin{cases} u_{n+1} = u_n + \lambda \Delta t u_n, n=0,1,2,\dots \\ u_0 \end{cases}$ and $\begin{cases} \tilde{u}_{n+1} = \tilde{u}_n + \lambda \Delta t \tilde{u}_n, n=0,1,2,\dots \\ u_0 + \varepsilon \end{cases}$

Take the difference of these expressions:

$$\tilde{u}_{n+1} - u_{n+1} = \tilde{u}_n - u_n + \lambda \Delta t \tilde{u}_n - \lambda \Delta t u_n$$

($\tilde{u}_{n+1}$: at $t = t_{n+1}$)

$$= (1 + \lambda \Delta t)(\tilde{u}_n - u_n)$$

$$= (1+\lambda \Delta t)(1+\lambda \Delta t)(\tilde{u}_{n-1} - u_{n-1})$$

$$= (1+\lambda \Delta t)(1+\lambda \Delta t)(1+\lambda \Delta t)(\tilde{u}_{n-2} - u_{n-2})$$

$$= \cdots$$

$$= (1 + \lambda \Delta t)^{n+1} \cdot (\tilde{u}_0 - u_0)$$

$$= (1+\lambda \Delta t)^{n+1} \cdot \varepsilon$$

(ε: "small" choice; $1+\lambda \Delta t$: in DE)

Remark: If $|1+\lambda \Delta t| < 1$, then the perturbation at $t = t_{n+1}$ remains "small", or even becomes smaller.
$\Leftrightarrow$ a stable numerical solution

If $|1+\lambda \Delta t| > 1$, then the perturbation at $t = t_{n+1}$ "blows up".
$\Leftrightarrow$ an unstable numerical solution

$$-1 < 1+\lambda \Delta t < 1 \Leftrightarrow -2 < \lambda \Delta t < 0$$
$$\Leftrightarrow \lambda \Delta t > -2$$

($\lambda \Delta t < 0$: always satisfied !! $\Delta t > 0, \lambda < 0$ (not interesting); $\lambda < 0$; $\Delta t > 0$)

example $\lambda = -10^8$ (in chemical reaction DEs, for example)
$\Leftrightarrow$ num. sol stable $\Delta t < 2 \cdot 10^{-8}$ (very very ... small)

An alternative method, based on the "other" "lim definition" of u' (see earlier):

$\lim_{\Delta t \to 0}$

$u'(t) = \lim_{\Delta t \to 0} \frac{u(t) - u(t-\Delta t)}{\Delta t}$

Euler-Backward (EB) or Implicit Euler

accuracy: $cst * \Delta t \sim EF$

$$u_{n+1} = u_n + \Delta t \cdot f(u_{n+1}, t_{n+1})$$

u_{n+1}: previous value; u_n: choice; $f(u_{n+1}, t_{n+1})$: known

Applied to the two (unperturbed and perturbed) test models:

$$\Longrightarrow \tilde{u}_{n+1} - u_{n+1} = \frac{1}{1-\lambda\Delta t}(\tilde{u}_n - u_n)$$ check!

$$\Longrightarrow \tilde{u}_{n+1} - u_{n+1} = \frac{1}{(1-\lambda\Delta t)^{n+1}}\varepsilon$$ ← small

$\frac{1}{(1-\lambda\Delta t)^{n+1}}$ always < 1

$\Rightarrow$ always (numerically) stable !!!

Disadvantage of EB:

$$u_{n+1} - \Delta t\, f(u_{n+1}, t_{n+1}) - u_n = 0$$

u_{n+1}: choice; f: nonlinear; u_{n+1}, t_{n+1}: known

$\Longrightarrow u_{n+1} = ???$

how? — we need Newton-Raphson in each step from t_n to t_{n+1} (finding a zero of the function on the left of the = sign)

How to apply to Hamiltonian DEs ?

example : $q'' + \sin(q) = 0$ (pendulum with $m=1, l=1, "g"=1$)

$\Leftrightarrow \begin{cases} q' = p \\ p' = -\sin(q) \end{cases}$

Note " $''$ " can also be written as " $\cdot\cdot$ "

$\mathcal{H}(q,p) = \frac{1}{2}p^2 - \cos(q)$ (energy)

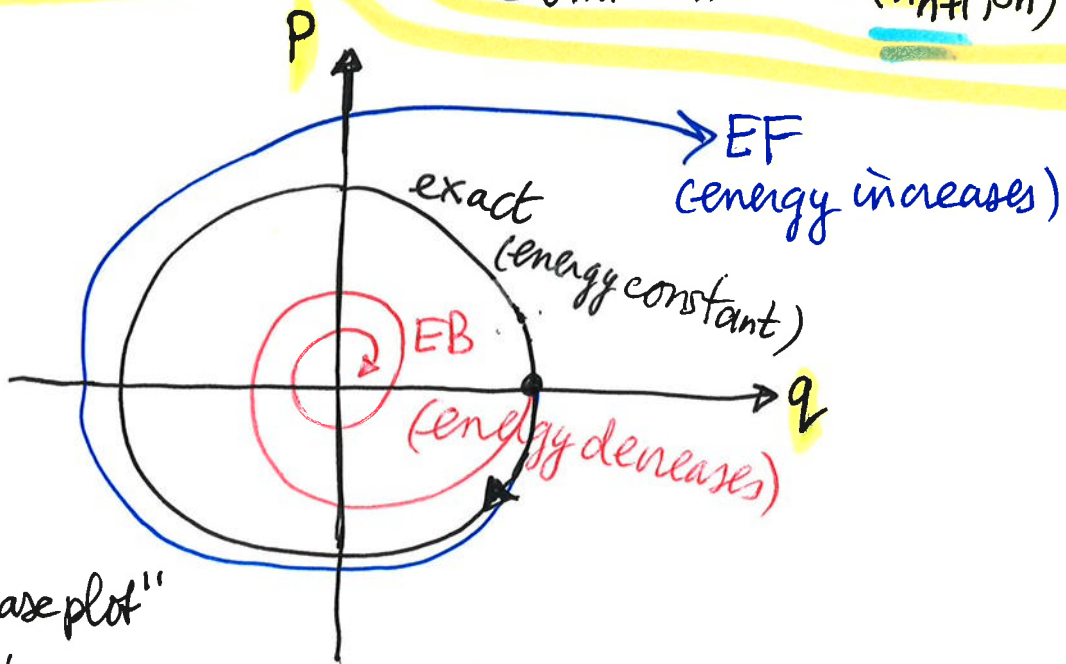
more general system of two DEs:

$$\begin{cases} x' = a(x,y) \\ y' = b(x,y) \end{cases}$$

EF: $\begin{cases} x_{n+1} = x_n + \Delta t \cdot a(x_n, y_n) \\ y_{n+1} = y_n + \Delta t \cdot b(x_n, y_n) \end{cases}$

EB: $\begin{cases} x_{n+1} = x_n + \Delta t \cdot a(x_{n+1}, y_{n+1}) \\ y_{n+1} = y_n + \Delta t \cdot b(x_{n+1}, y_{n+1}) \end{cases}$

Sympletic Euler: $\begin{cases} x_{n+1} = x_n + \Delta t \cdot a(x_n, y_n) \\ y_{n+1} = y_n + \Delta t \cdot b(x_{n+1}, y_n) \end{cases}$



"phase plot"

(time t varies on each curve)

Störmer-Verlet method

$q'' = f(q)$ [or as a system with a Hamiltonian that should be constant in time t $\Leftrightarrow \frac{dH}{dt} = 0$]

numerical solution → approximate q'' (instead of q' as before)

↕ see exercise in tutorial (via Taylor)

$$\frac{q_{n+1} - 2q_n + q_{n-1}}{(\Delta t)^2} = f(q_n), \quad n = 1, 2, 3, \dots, N-1$$

$$\Leftrightarrow \quad q_{n+1} = 2q_n - q_{n-1} + (\Delta t)^2 f(q_n)$$

↑ we need two starting values!

q_0 is given, $q_1 = ?$ $\Rightarrow q_2 = \dots$, $q_3 = \dots$, ⋮

$$q_1 = q_0 + \Delta t\, q_0' + \frac{(\Delta t)^2}{2} q_0'' \quad (+ \dots) \qquad \text{"Taylor"}$$

$q_0' = v_0$ (initial velocity); neglect; $q_0'' = f(q_0)$

Other variants exist ↔ velocity-Verlet ↔ ...