Numerical optimization

$$f : \vec{x} \in \mathbb{R}^N \to f(\vec{x}) \in \mathbb{R}$$

continuous variables

$$f : \vec{\sigma} \to f(\vec{\sigma}) \in \mathbb{R}$$

$$\vec{\sigma} = (\sigma_1, \sigma_2, \ldots, \sigma_N) \quad \text{(Ising spins)}$$

$$\sigma_i = \pm 1 \quad \text{Ising variable (binary variable)}$$

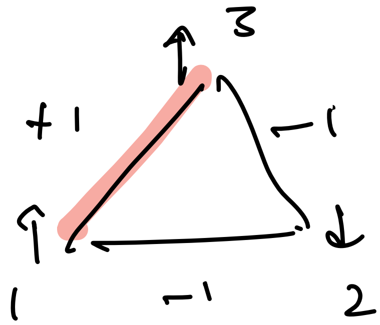
Find the minimum of f $\quad \sigma^2 = 1$

magnetic field $\qquad$ two-spin int.

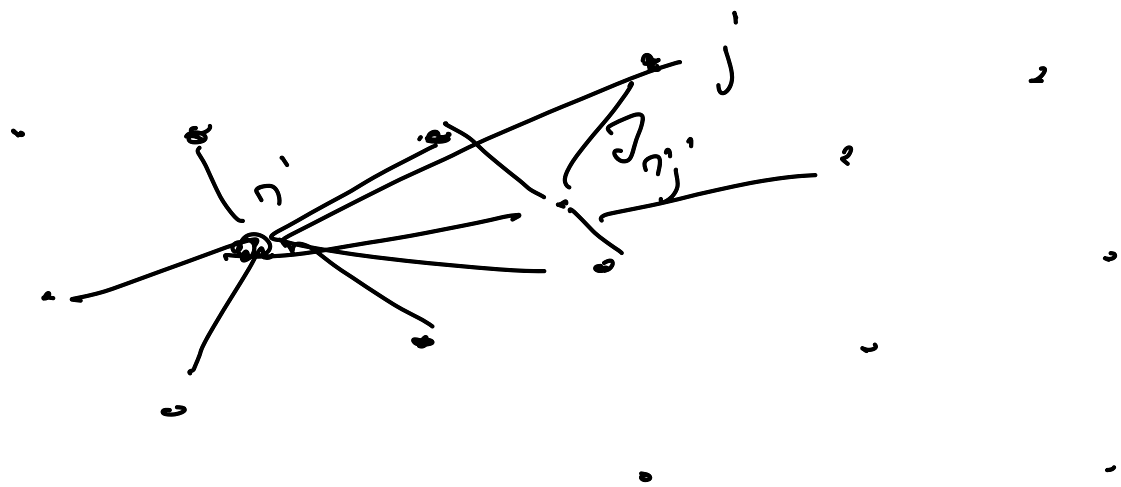
$$f(\vec{\sigma}) = -\sum_{i=1}^{N} h_i \sigma_i + \sum_{ij} J_{ij} \sigma_i \sigma_j + \sum_{ijl} K_{ijl} \sigma_i \sigma_j \sigma_l + \ldots$$

$\#$ of configs : 2^N

"Frustrated" (competing) interactions



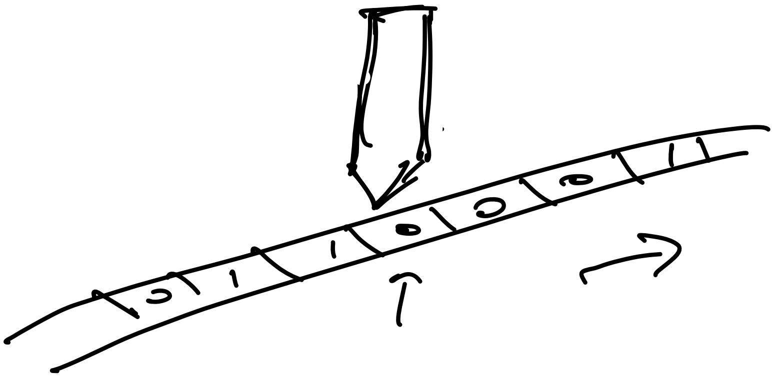
$$f = \sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1$$



randomness + frustration $\Rightarrow$ hardness of minimization ?

Primer in computational complexity

1) Deterministic Turing machine (DTM)

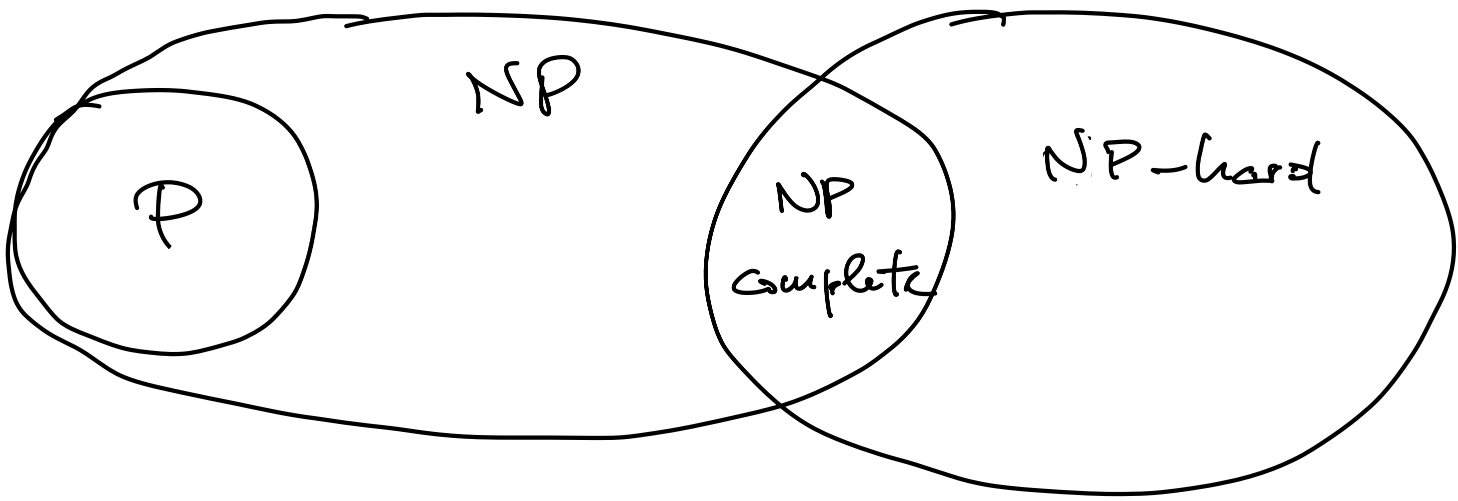


2) Non-deterministic Turing machine (NTM)

at every step → write 1 with prob p

→ write 0 with prob. $1-p$

Complexity classes $P \subset NP$?



P: ensemble of problems solvable in poly time by a DTM

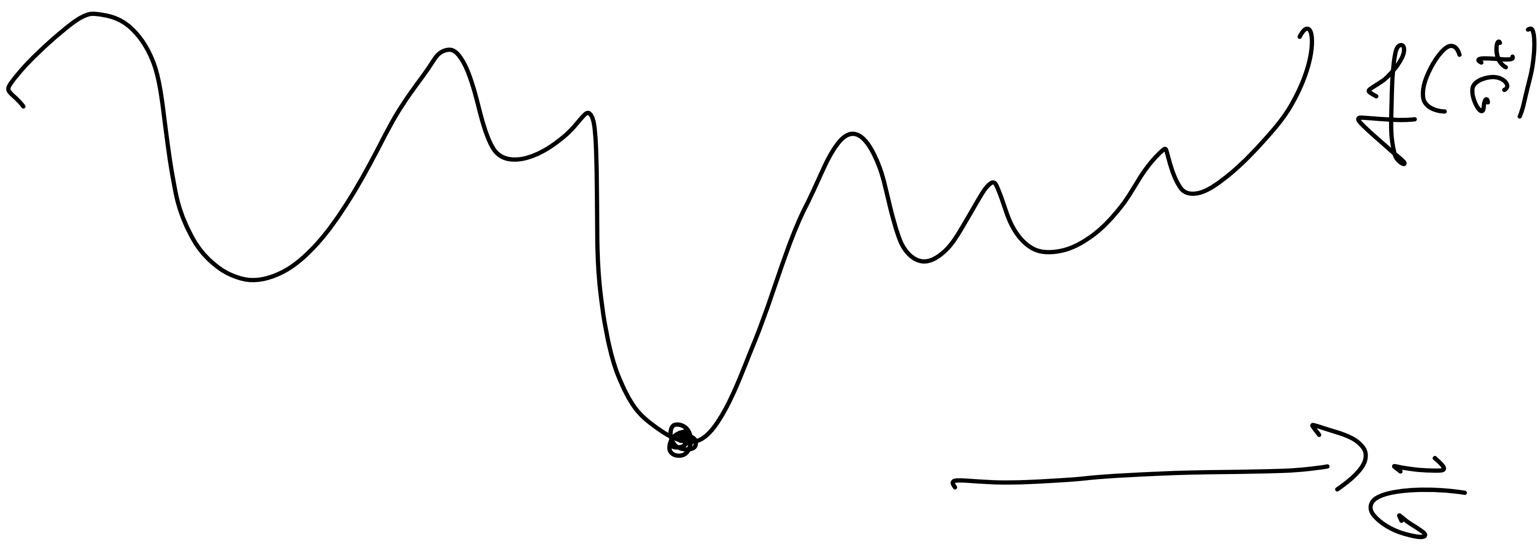
NP: (1) ensemble of problems solvable in poly time by a NTM –

(2) the solution can be checked in poly time by a DTM

NP-hard : ① ~~②~~

all problems in NP can be mapped in polynomial time as problems in NP-hard

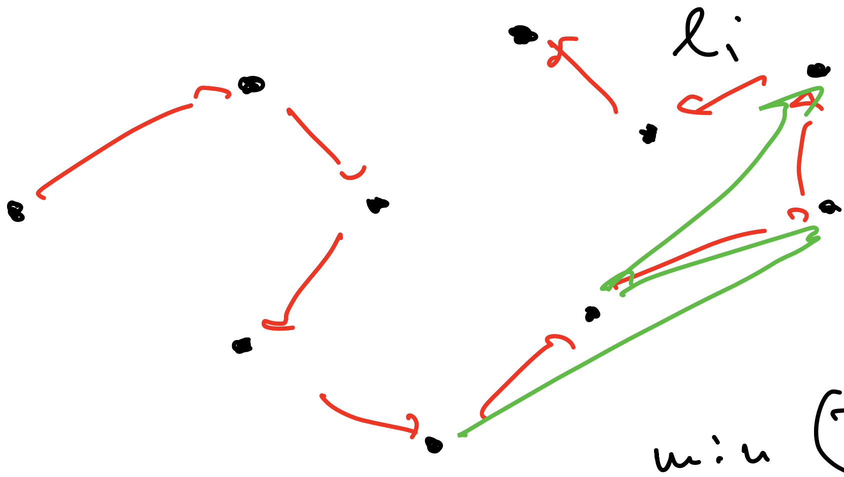
There are optimization problems that can be proven to be NP-hard



NP-complete : Boolean satisfiability

(a or b) and (b or c) and . _

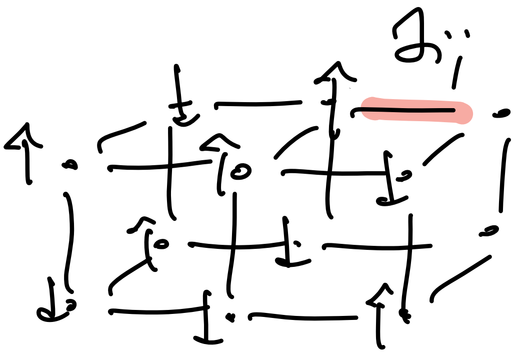
NP-hard : traveling salesman problem



$\rightarrow$ $\min\left(\sum_i l_i\right)$

Physics : minimization of the energy of Ising models (spin glasses)

ex. :



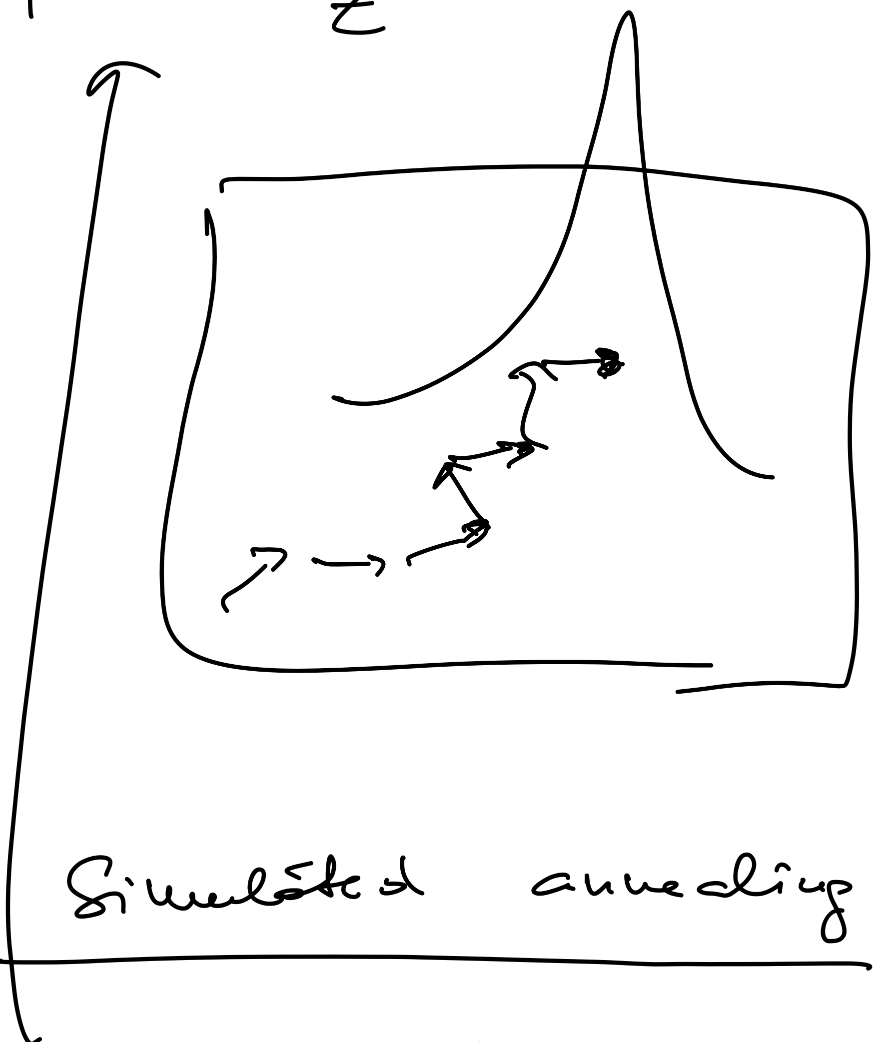
$\Rightarrow$ $J_{ij} = (0, -1, +1)$ random

$\rightarrow$ $E(\sigma) = \sum_{ij} J_{ij}\, \sigma_i \sigma_j$

ED NP-hard

$$p_T(\vec{\sigma}) = \frac{e^{-E(\vec{\sigma})/T}}{Z}$$

$$Z = \sum_{\vec{\sigma}} e^{-E(\vec{\sigma})/T}$$



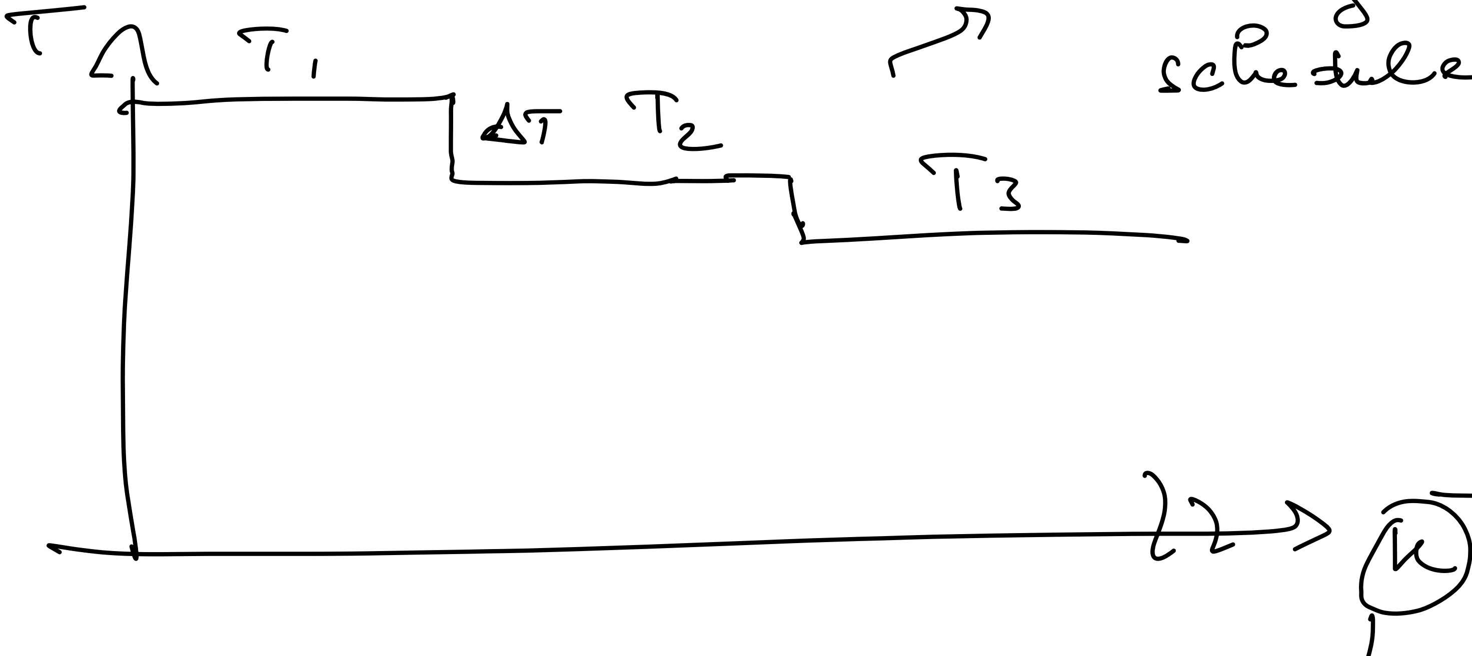
$T \to 0$

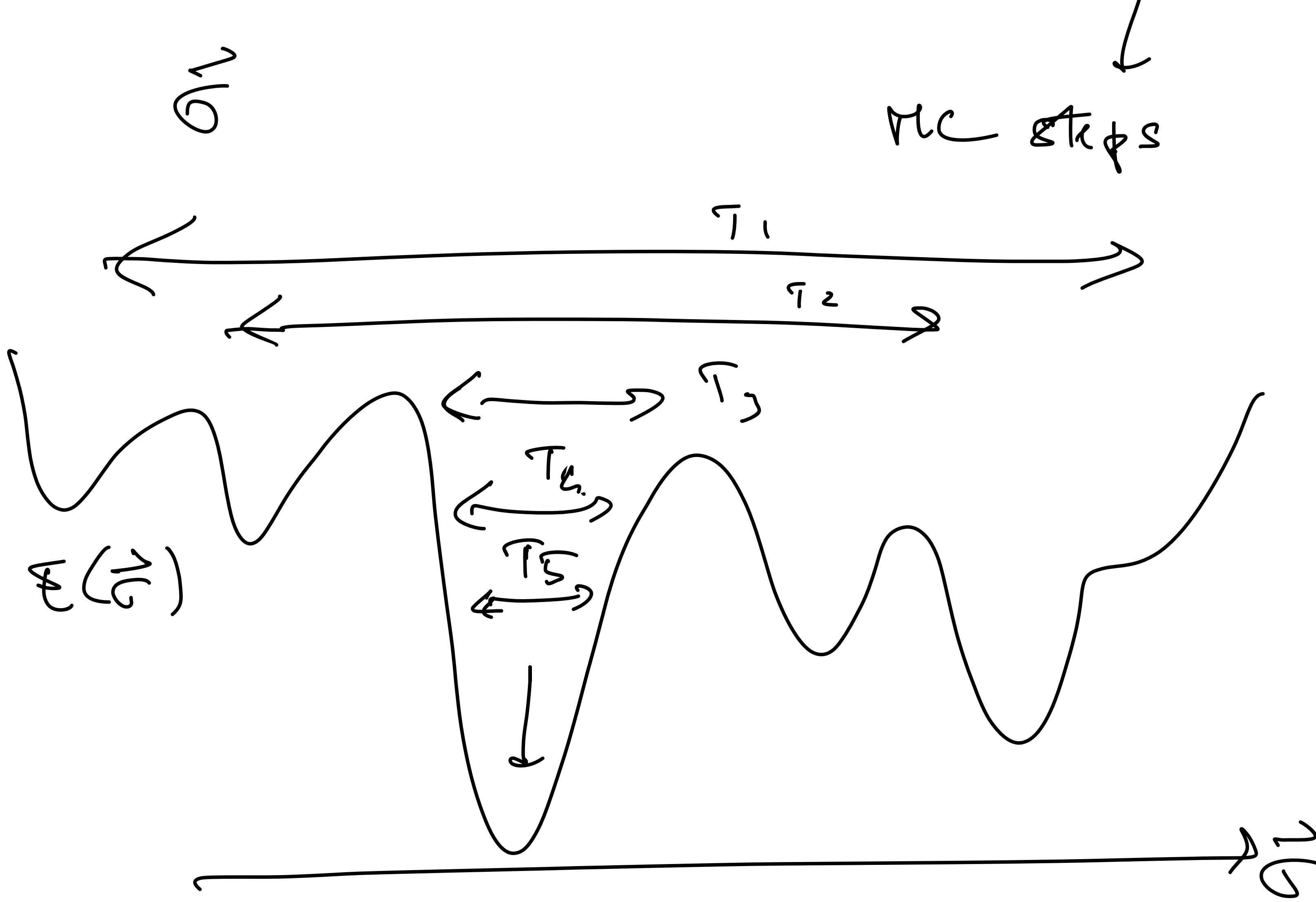
$\vec{\sigma}$

Simulated annealing

MC simulation

"annealing schedule"





When $\underline{\underline{E(\vec{\sigma})}}$ is a model of an Ising spin glass

$E \to L = \sum_i l_i$

$$p(\{l_i\}) = \frac{e^{-(\sum_i l_i)/T}}{Z}$$

Problem : $\tau \sim O(\exp(N))$

τ : autocorrelation times

Proof of efficiency for simulated annealing :

you are guaranteed to get to the absolute minimum by using an annealing schedule

$$T_k \simeq \frac{cN}{\log k}$$

$$k = \exp\left(\frac{cN}{T}\right)$$

Numerical solution of ODEs

$$\Rightarrow \vec{x}(t) = (x_1(t), x_2(t), \ldots, x_N(t))$$

$$\vec{F}(\vec{x}, \dot{\vec{x}}, \ddot{\vec{x}}, \ldots, \vec{x}^{(m)}; t) = 0$$

$\underline{m\text{-th order ODE}}$

ordinary differential equation

1-st order $\underline{\text{ODE}}$

$$\vec{q}_1(t) = \vec{x}(t)$$

$$\vec{q}_2 = \dot{\vec{x}}$$

$$\vec{q}_3 = \dot{\vec{q}}_2 = \ddot{\vec{x}}$$

$$\vdots$$

$$\vec{q}_m = \vec{x}^{(m-1)} = \dot{\vec{q}}_{m-1}$$

$$\vec{G}(\underbrace{\vec{q}_1, \vec{q}_2, \vec{q}_3, \ldots; \vec{q}_m}_{\vec{q}}; \underbrace{\dot{\vec{q}}_1, \dot{\vec{q}}_2, \ldots, \dot{\vec{q}}_m}_{\dot{\vec{q}}}; t) = 0$$

$$\underline{\vec{G}(\vec{q}, \dot{\vec{q}}, t) = 0}$$

Cauchy problem

$$\boxed{\begin{cases} \dot{\vec{q}} = \vec{f}(\vec{q}(t), t) \\ \vec{q}(0) = \vec{q}_0 \end{cases}}$$

$\rightarrow$ initial conditions

Ex.: Newton's equations

$$m\ddot{\vec{x}}(t) = \vec{F}(\vec{x}(t), t)$$

$$\vec{q}_1(t) = \vec{x}(t)$$
$$\vec{q}_2(t) = \dot{\vec{x}}(t)$$

$$\begin{cases} \dot{\vec{q}}_1 = \vec{q}_2 \\ \dot{\vec{q}}_2 = F(\vec{q}_1, t) \end{cases}$$

Numerical solution to a Cauchy problem comes with a finite accuracy

$$|\vec{y}_{num}(t) - \vec{y}_{exact}(t)| \leq \epsilon$$

$$t \in [0, t_0]$$

time to solution with accuracy ϵ

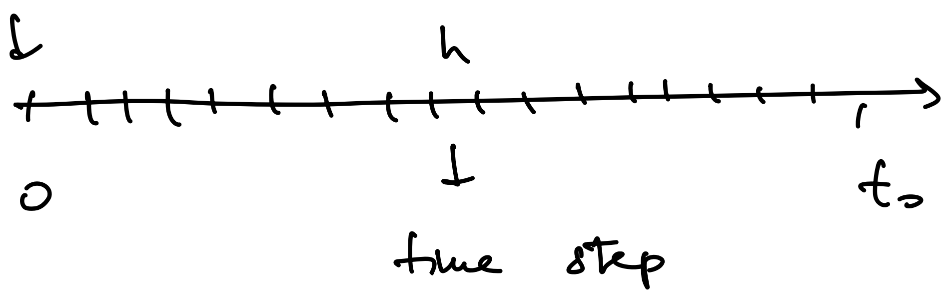
$$T = A \frac{N}{\epsilon^{\alpha}}\left(\frac{t_0}{\vartheta}\right)$$

general scaling

$$\alpha \sim o(1)$$

Numerical scheme of integration

in general it goes via discretization of time



$$\vec{q}(t) \rightarrow \vec{q}_n \simeq \vec{q}(t_n)$$

$$t_n = nh$$

numerical scheme : explicit

$$\vec{q}_{n+1} = \vec{\mathcal{Y}}_n(\vec{q}_n, \vec{q}_{n-1}, \vec{q}_{n-2}, \ldots, \vec{q}_0 ; h)$$

$$=$$

implicit

$$\vec{q}_{n+1} = \vec{\mathcal{Y}}_n(\vec{q}_{n+1}, \vec{q}_n, \vec{q}_{n-1}, \ldots, \vec{q}_0 ; h)$$

Special case : time-independent linear set of ODEs

$$\dot{\vec{q}}(t) = A\vec{q} \qquad \vec{q}(0) = \vec{q}_0$$

$$\Rightarrow \vec{q}(t) = e^{At}\vec{q}_0$$

A symmetric $\rightarrow$ $U^T A U = \mathrm{diag}(\lambda_1, \ldots, \lambda_N)$

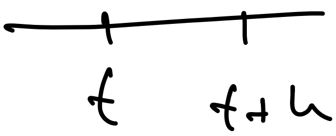
$$e^{At} = U^T \mathrm{diag}(e^{\lambda_1 t}, e^{\lambda_2 t}, \ldots, e^{\lambda_N t})\, U$$

How do you build an <u>integration scheme</u> ?

$$\dot{\vec{q}}(t) = \vec{f}(\vec{q}; t)$$

$$\int_t^{t+h} \dot{\vec{q}}(t)\, dt = \vec{q}(t+h) - \vec{q}(t)$$

$$= \underbrace{\int_t^{t+h} dt' \, \vec{f}(\underline{\vec{q}(t')}; t')}$$



if h is small

expand $\vec{q}(t')$ around $\vec{q}(t)$

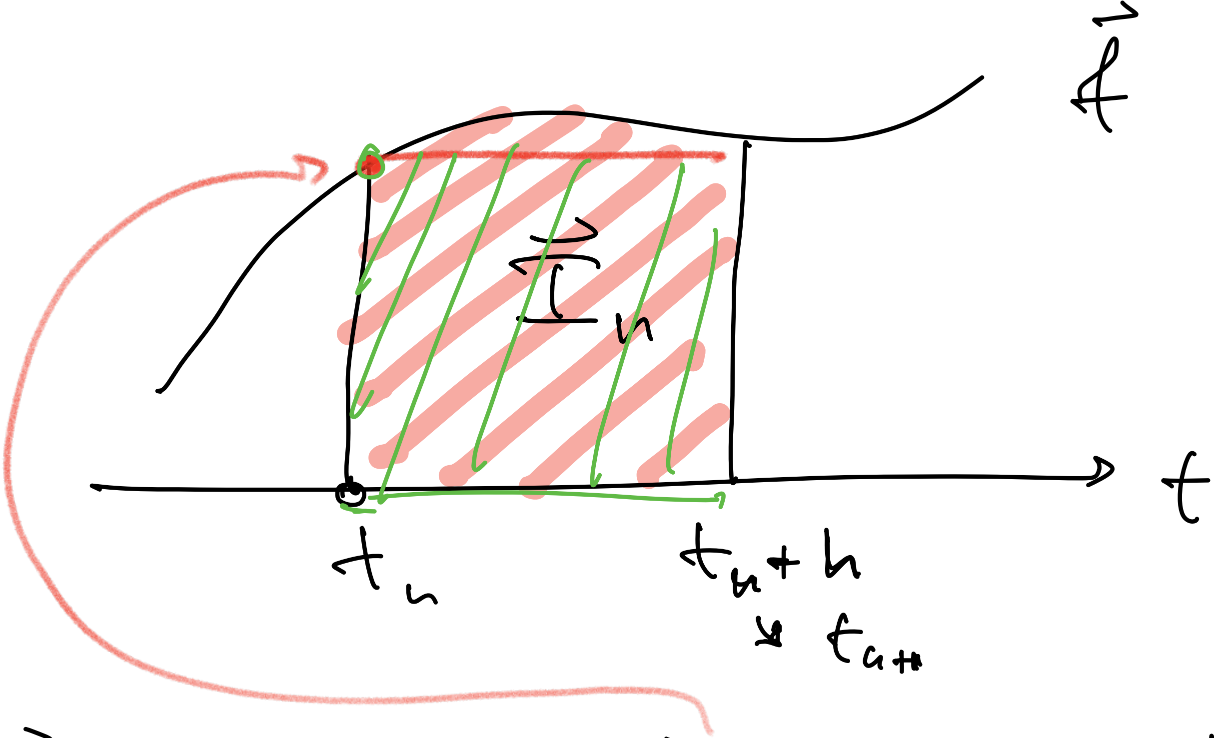
$$\simeq \int_t^{t+h} dt' \left[\vec{f}(q(t); t) + (t'-t) \frac{d\vec{f}}{dt} + \dots \right] \qquad O(t-t')^2$$

$$= \underline{h \vec{f}(\vec{q}(t), t) +} \ \frac{1}{2} h^2 \frac{d\vec{f}}{dt}(\vec{q}(t); t) + O(h^3)$$

$t \to t_n = nh$

$$\vec{q}_{\underline{n+1}} - \vec{q}_n = \int_{t_n}^{t_n+h} dt' \, \vec{f}(\vec{q}(t'); t')$$

$$= \vec{I}_n$$



$$\vec{y}_{n+1} - \vec{y}_n \simeq h\,\vec{f}(\vec{y}_n, t_n) + \frac{h^2}{2}\frac{d\vec{f}}{dt}(\vec{y}_n, t_n) + \dots$$

numerical integration scheme = good approximation of $\vec{I}_n$

<u>Euler method</u> (18th century)

$$\vec{y}_{n+1} \simeq \vec{y}_n + h\,\vec{f}(\vec{y}_n, t_n) + O(h^2)$$

$\uparrow$

Order of consistency of a numerical scheme

numerical scheme

$$\vec{y}_{n+1} = \vec{\mathcal{Y}}_n\left((\vec{y}_{n+1}), \vec{y}_n, \dots, \vec{y}_0; h\right)$$

"local" error

$$\vec{\eta}_{n+1} = \underbrace{\vec{y}(t_{n+1})}_{\text{exact sol.}} - \vec{\mathcal{Y}}_n\left((\vec{y}(t_{n+1})), \vec{y}(t_n), \dots, \vec{y}_0; h\right)$$

method is consistent of order p over an interval $[0, t_0]$

if $$\max_{n \in [1,\, t_0/h]} |\vec{\eta}_n| = h\,\tau(h)$$

$$\lim_{h \to 0} \tau(h) \sim h^p$$

error $\sim O(h^{p+1})$

Euler : error $\sim O(h^2)$

$\Rightarrow$ $\underline{p = 1}$

Convergence of a method

<u>global error</u>

$$\vec{\xi}_n = \vec{y}_n - \vec{y}(t_n)$$

method is convergent of order p if

$$\lim_{h \to 0} \left(\max_{n \in [0, t_f/h]} |\vec{\xi}_n| \right) \sim \underline{O(h^p)}$$

Simple idea:

$$\vec{y}_1 = \vec{y}(t_1) + O(h^{p+1})$$

$$\vec{y}_2 = \vec{y}(t_2) + 2\,O(h^{p+1})$$

$$\vdots$$

$$\vec{y}_n = \vec{y}(t_n) + n\,O(h^{p+1})$$

$$n = t_0/h$$

$$= \vec{y}(t_n) + t_0 O(h^p)$$

Euler can be proven to be consistent and convergent of <u>order 1</u>