Computational optimization, glasses & black holes :

A rare mix with many common features

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En tu honor, mami

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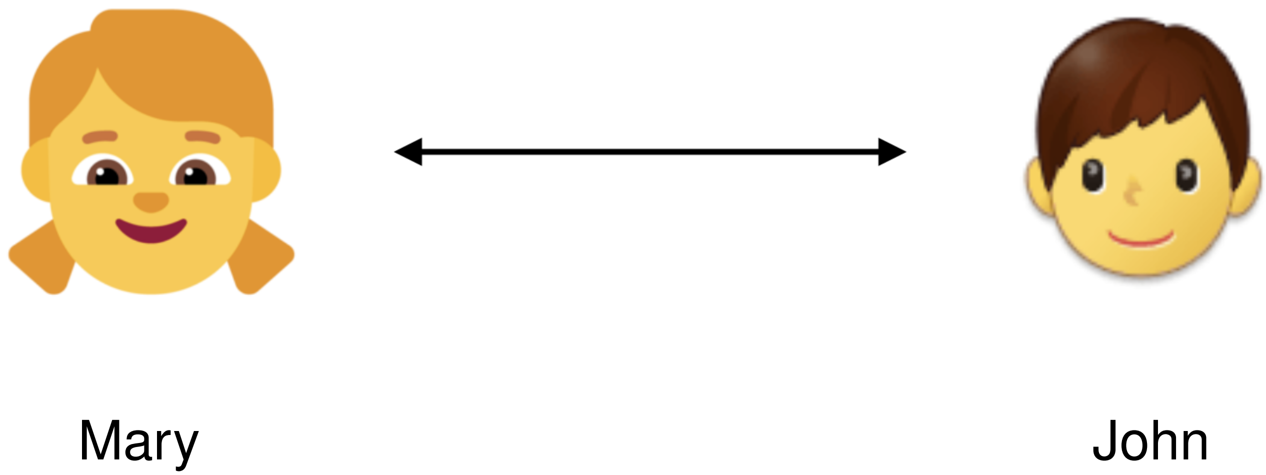
Computational optimisation

Setting

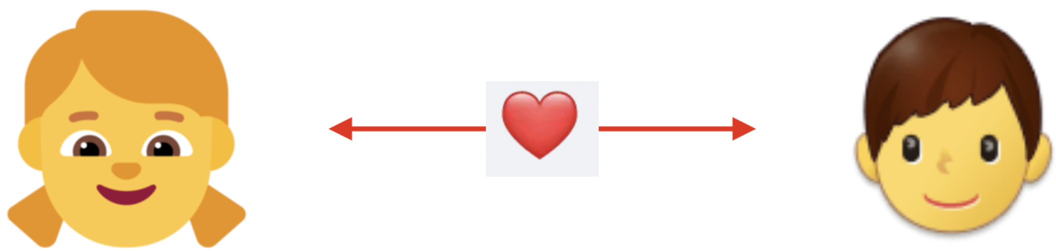
Take two individuals



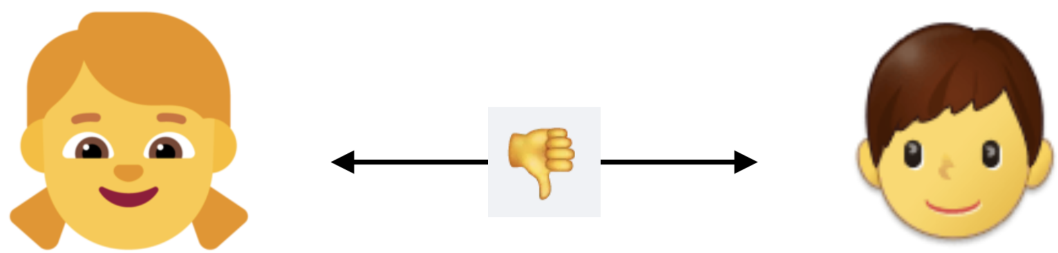
They may like or dislike each other

Setting

Identify their feelings towards each other



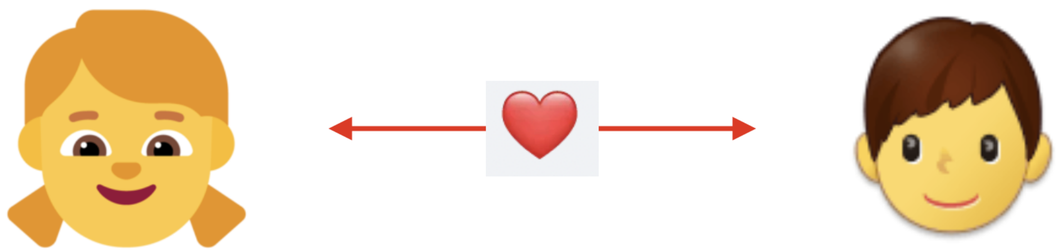
or



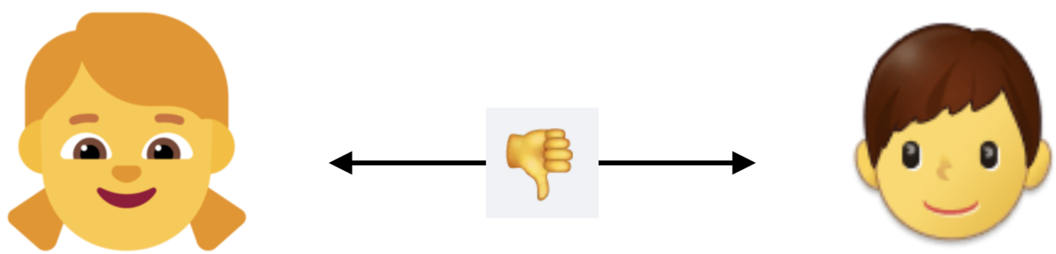
Assume they are reciprocal

Setting

Define a pairwise interaction



$$J_{\text{Mary}-\text{John}} = -1$$



$$J_{\text{Mary}-\text{John}} = +1$$

An easy problem

Going out for dinner in a group of three

You ❤️ Mary

You ❤️ John

Mary ❤️ John

Happy dinner

An easy problem

Going out for dinner : give a score

You	❤️	Mary	-1
You	❤️	John	-1
Mary	❤️	John	-1

Happy dinner $\boxed{-3}$

The rule is to add $J = -1$ for each happy pair

Easy vs. constrained

Going out for dinner in a group of three

You	❤️	Mary	-1
You	❤️	John	-1
Mary	❤️	John	-1
Happy dinner			$\boxed{-3}$

You	❤️	Mary	-1
You	❤️	John	-1
Mary	👎	John	$+1$
Conflicting dinner			$\boxed{-1}$

The rule is to add $J = -1$ for each happy pair or $J = +1$ for each unhappy one

Easy vs. constrained

Define a cost function

You	❤️	Mary	-1
You	❤️	John	-1
Mary	❤️	John	-1

Happy dinner $\boxed{-3}$

You	❤️	Mary	-1
You	❤️	John	-1
Mary	👎	John	$+1$

Conflicting dinner $\boxed{-1}$

The rule is to add $J = -1$ for each happy pair and $J = +1$ for each unhappy one

The **cost function** takes a **higher value** when there is **frustration**

An optimisation problem

Change the proposal : split the group in two

Three cases

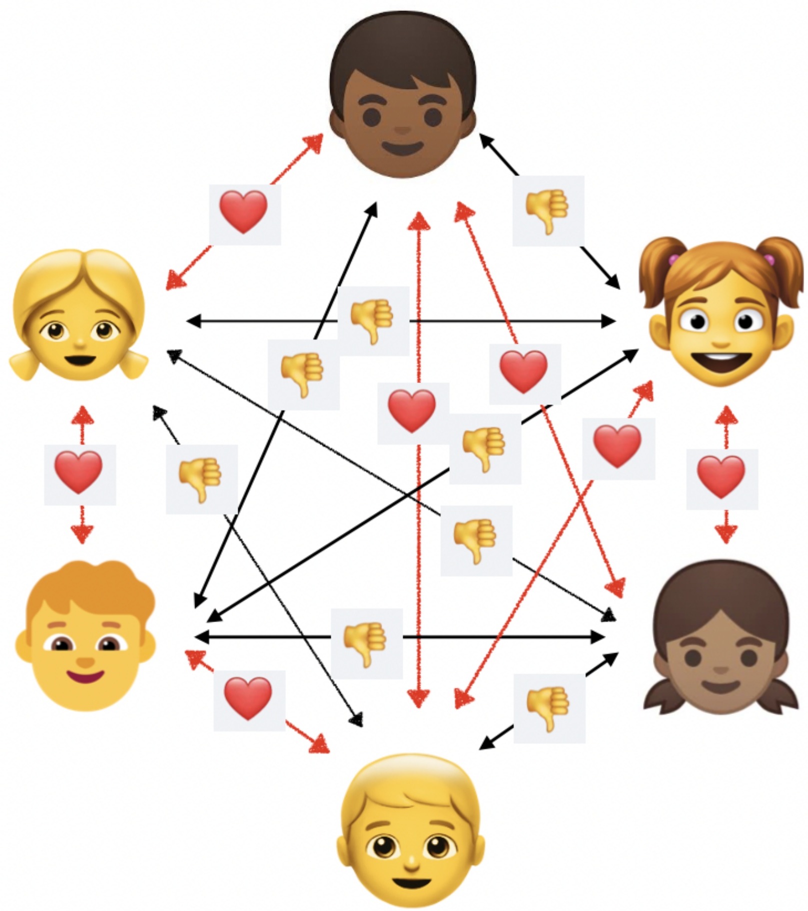
(You & Mary ❤️ go out)	(John is not invited)	✔	-1
(You & John ❤️ go out)	(Mary is not invited)	✔	-1
(Mary & John 👎 go out)	(You are not invited)	✘	$+1$

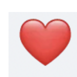
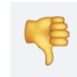
The value of the cost function is the J of the couple

There are two **optimal** solutions which **minimize** the **cost function**

An optimisation problem

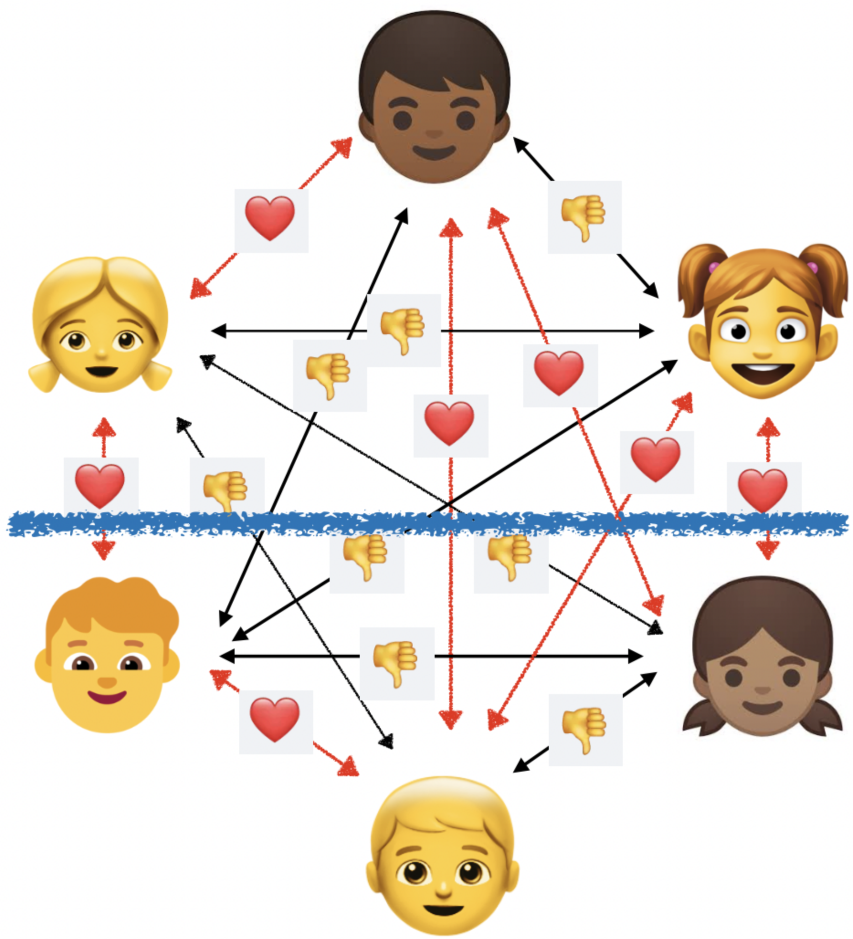
More people, many more connections, complexity increases



Say that, roughly, half and half love  or hate  each other

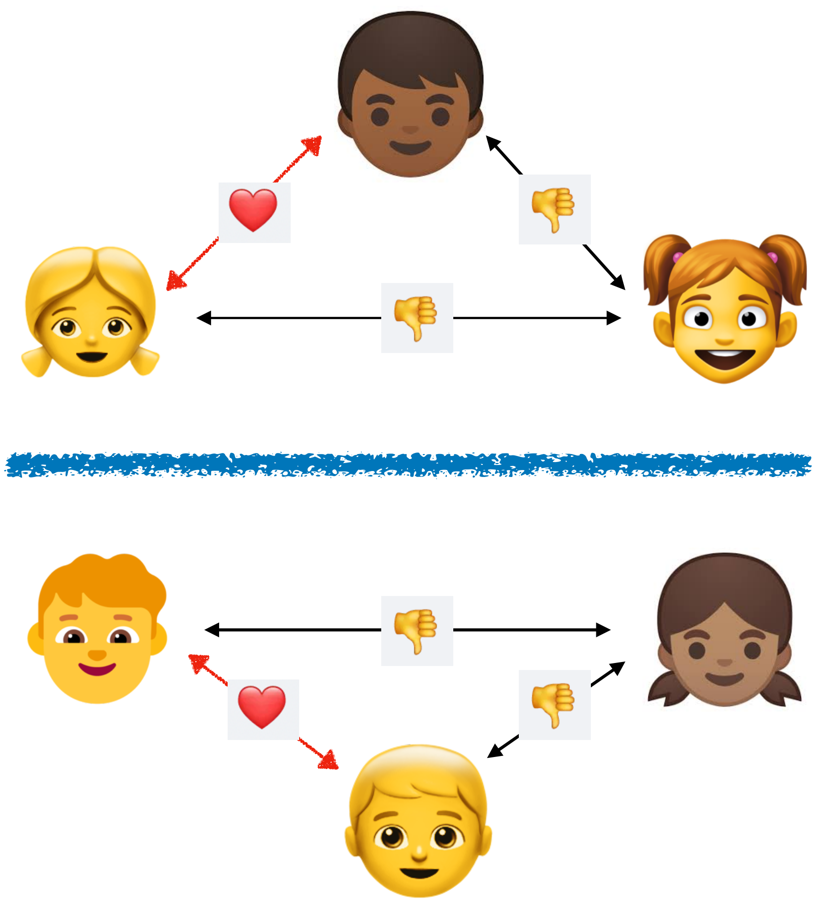
An optimisation problem

How do we split the group equally (& make two parties)?



An optimisation problem

Evaluate the cost function



Group A

Add -1 for ❤️ & $+1$ for 👎

Cost $_A = -1 + 1 + 1 = +1$

Group B

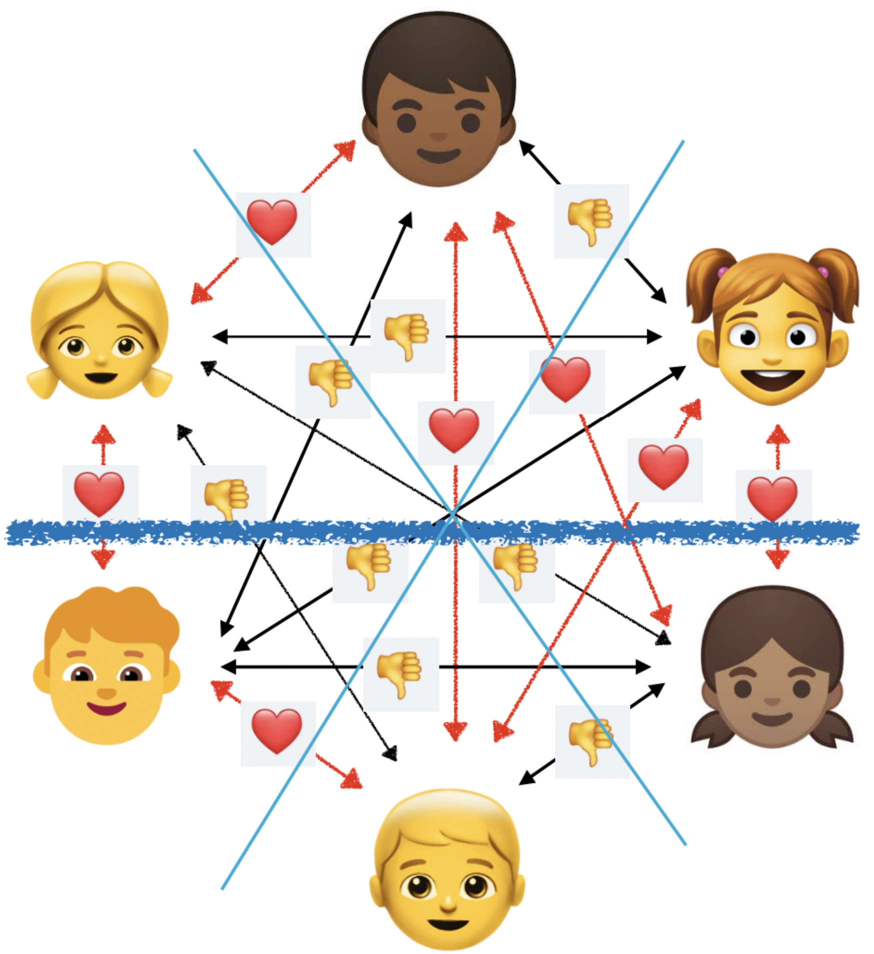
Add -1 for ❤️ & $+1$ for 👎

Cost $_B = -1 + 1 + 1 = +1$

The total cost is $C = C_A + C_B = 2$ **Is it a good solution ?**

An optimisation problem

Which is the optimal partition ? A hard problem



One can try all possible cuts for a few persons but not for many !

Mathematical representation

Setting the problem in a form amenable to calculations

Cost function

Just one equation (and quickly back to drawings)

In the **graph partitioning** - **group splitting** example

It is inconvenient to call the people by their name, we prefer to use number labels

Mary = 1 John = 2 Peter = 3 . . .

i labels the persons and runs from 1 to N, their total number

$\boxed{i = 1, \ldots, N}$ label the persons. For ex. $i = 1$ is Mary, $i = 2$ is John, etc.

Cost function

Just one equation (and quickly back to drawings)

In the **graph partitioning** - **group splitting** example

$i, j = 1, \ldots, N$ label the persons. For ex. $i = 1$ is Mary, $i = 2$ is John, etc.

Each pair of individuals in the group like or dislike each other

Mary and John like ❤️ each other $J_{\mathrm{Mary-John}} = J_{12} = -1$ while

Mary and Peter dislike 👎 each other $J_{\mathrm{Mary-Peter}} = J_{13} = +1$

and we call $\boxed{J_{ij}}$ the $N(N-1)/2$ frozen interactions - quenched disorder

Cost function

Just one equation (and quickly back to drawings)

In the **graph partitioning** - **group splitting** example

$i = 1, \ldots, N$ or $j = 1, \ldots, N$ label the persons

Each pair has a predetermined interaction

$J_{ij} = -1$ if love ❤️ or $J_{ij} = +1$ if hate 👎 between i and j

---

We set the value of a variable attributed to each person to

$\boxed{s_i = +1}$ if i is in group A or $\boxed{s_i = -1}$ if i is in group B

It characterises the state of the ith person

for ex. if Mary (labelled $i = 1$) is in group A, $s_{\text{Mary}} = s_1 = +1$

if John (labelled $i = 2$) is in group B, $s_{\text{John}} = s_2 = -1$

Cost function

Just one equation (and quickly back to drawings)

In the **graph partitioning** - **group splitting** example

$s_i = +1$ if i is in group A or $s_i = -1$ if i is in group B

Condition, equal-size groups

To ensure equal-size groups $\underbrace{s_1 + s_2 + \cdots + s_N} = 0$ (as many $+1$ as -1)

Short-hand notation $\sum_{i=1}^{N} s_i = 0$

represents a sum of the states of all people given by the values of the s_i

Cost function

Just one equation (and quickly back to drawings)

In the **graph partitioning** - **group splitting** example

$s_i = 1$ if i is in group A or $s_i = -1$ if i is in group B

find the assignment of the $\{s_i\}$ so that they **add up to zero** ($\sum_{i=1}^{N} s_i = 0$) & the

Cost function

$C =$ sum over all pairs — of the love/hate values — in the same group

is **minimised**

Cost function

Just one equation (and quickly back to drawings)

In the **graph partitioning** - **group splitting** example

$s_i = 1$ if i is in group A or $s_i = -1$ if i is in group B

find the assignment of all the s_i so that they **add up to zero** ($\sum_{i=1}^{N} s_i = 0$) & the

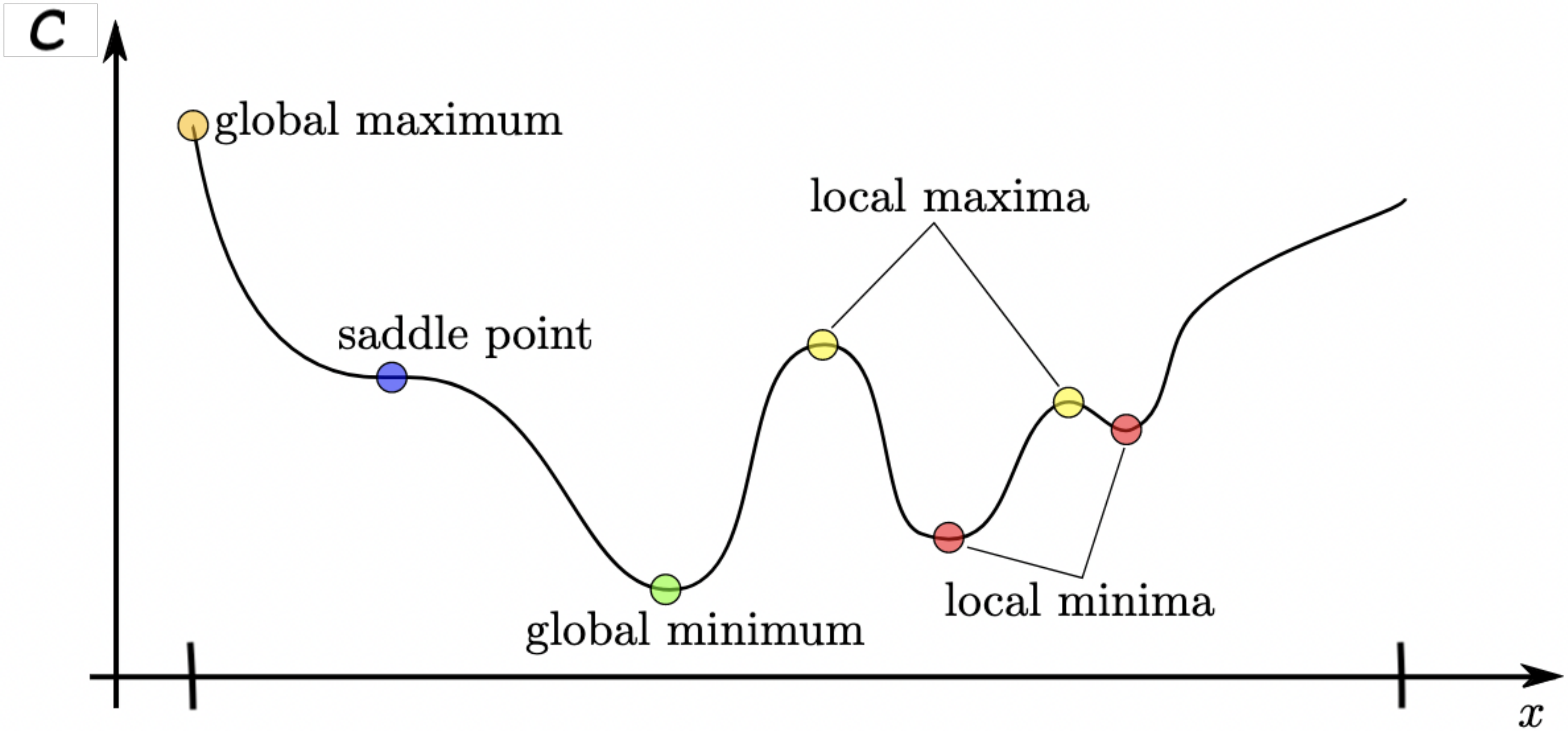
Cost function is minimised

$$C = \underbrace{\sum_{i \neq j}}_{\text{sum over all pairs}} \underbrace{J_{ij}}_{\text{love/hate}} \underbrace{\left(\frac{1 + s_i s_j}{2}\right)}_{\text{selects pairs in same group}}$$

vanishes if i, j in different groups

Cost function

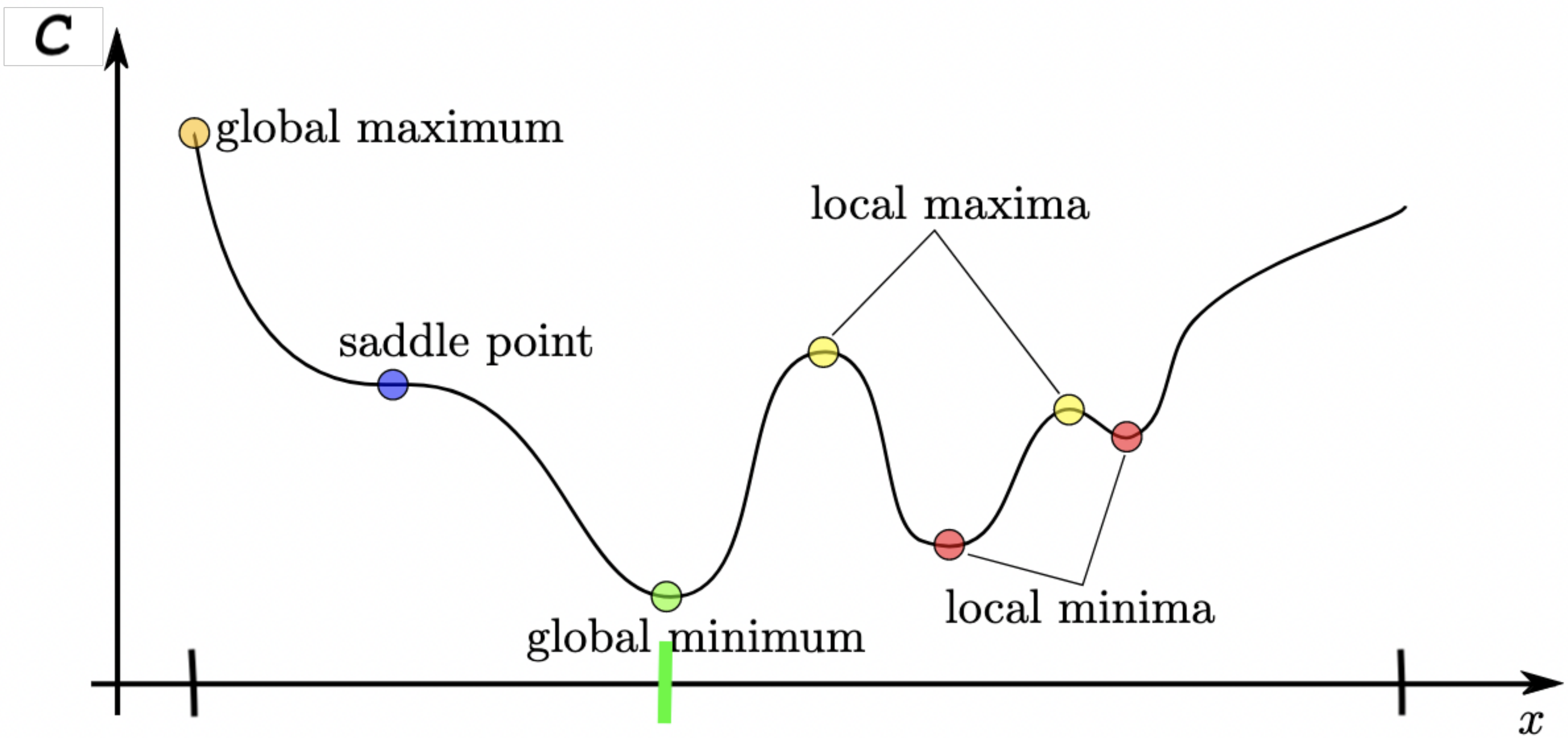
What is a function ? Think of a linear roller coaster



A real function C of a **single real variable** x

Cost function

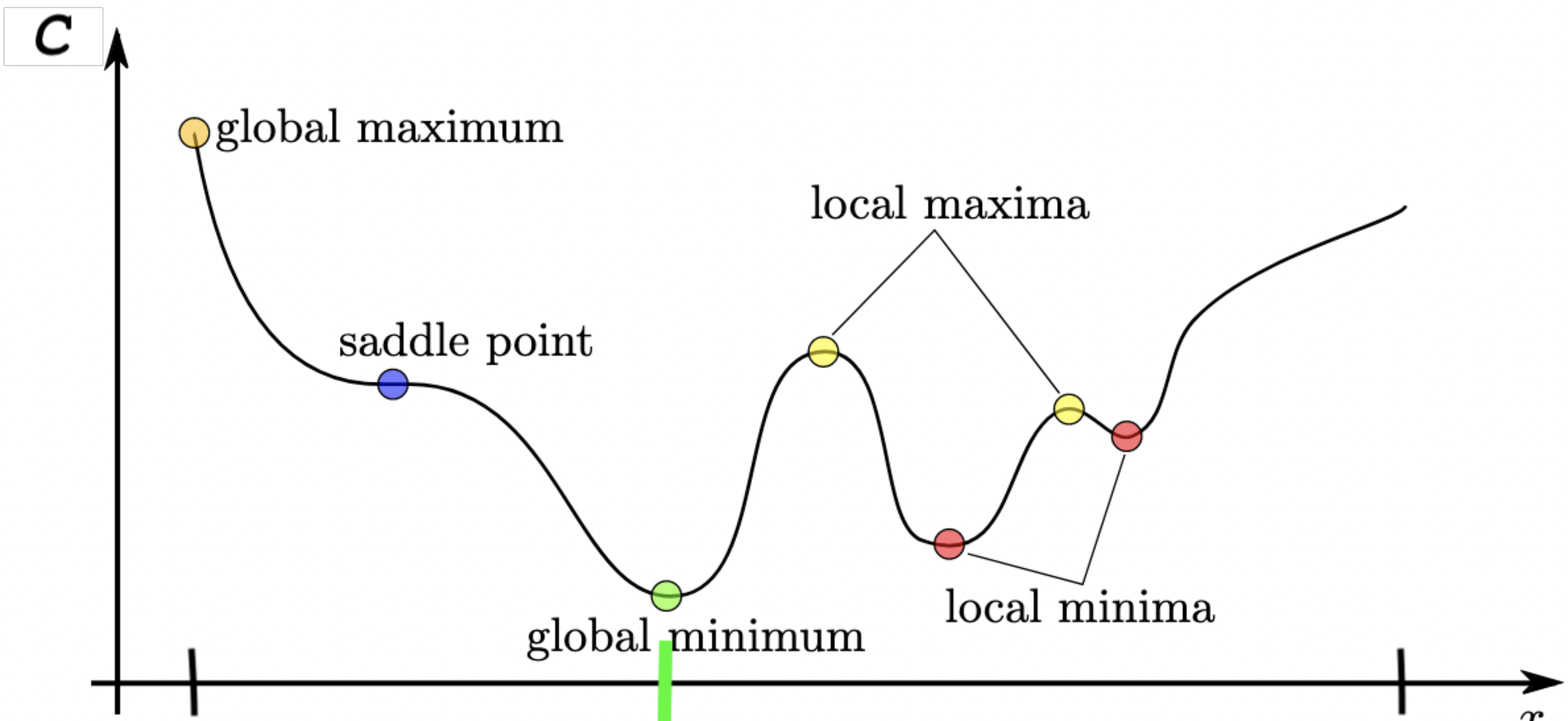
What is the goal ?



Find the absolute minimum x_{min}

Cost function

What is the goal ?



How does one move in this **landscape** to find x_{min} ?

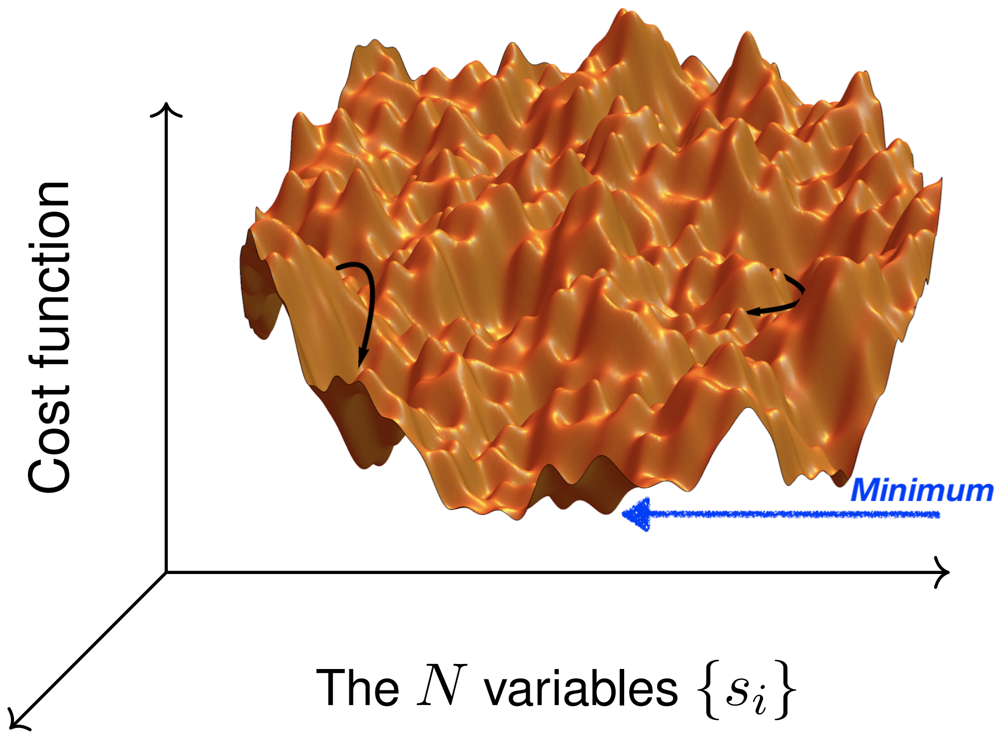
Think of a ball rolling down the slopes with some friction:

– if it starts from the right end, it'll end up in a local minimum x_{min}

– if it starts from the left end, it'll end up in the absolute minimum x_{min}

Cost function

Rugged landscape in a large dimensional space - a sketch

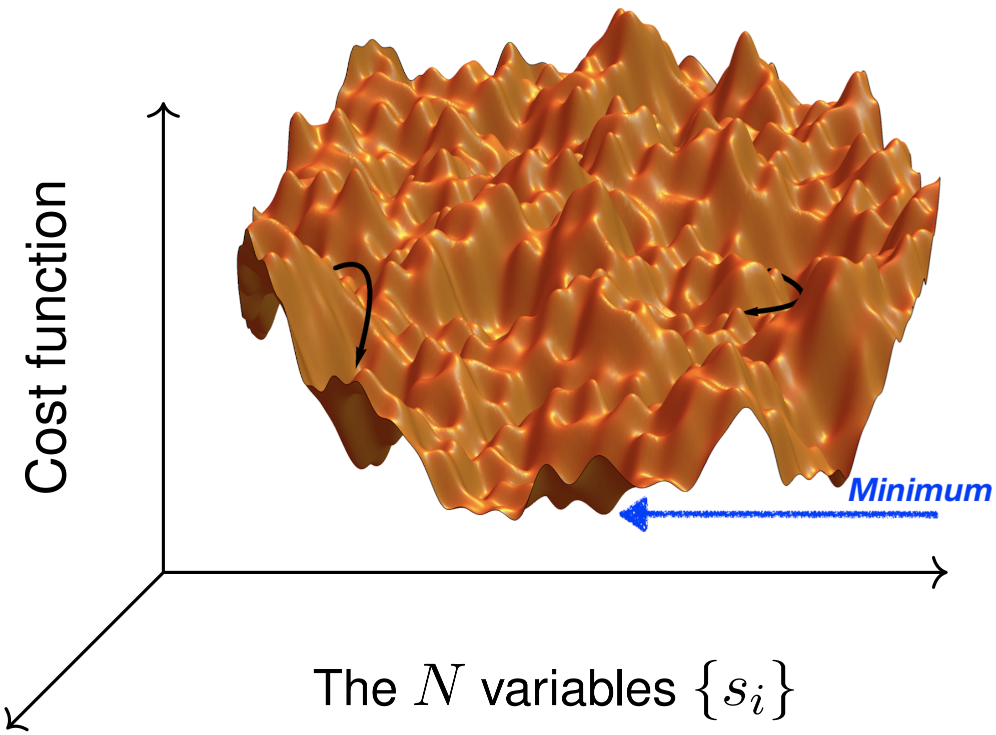


The lanscape is fixed by the $\{J_{ij}\}$ - quenched randomness

or disorder - for a typical realization of the problem

Cost function

Rugged landscape in a large dimensional space - a sketch

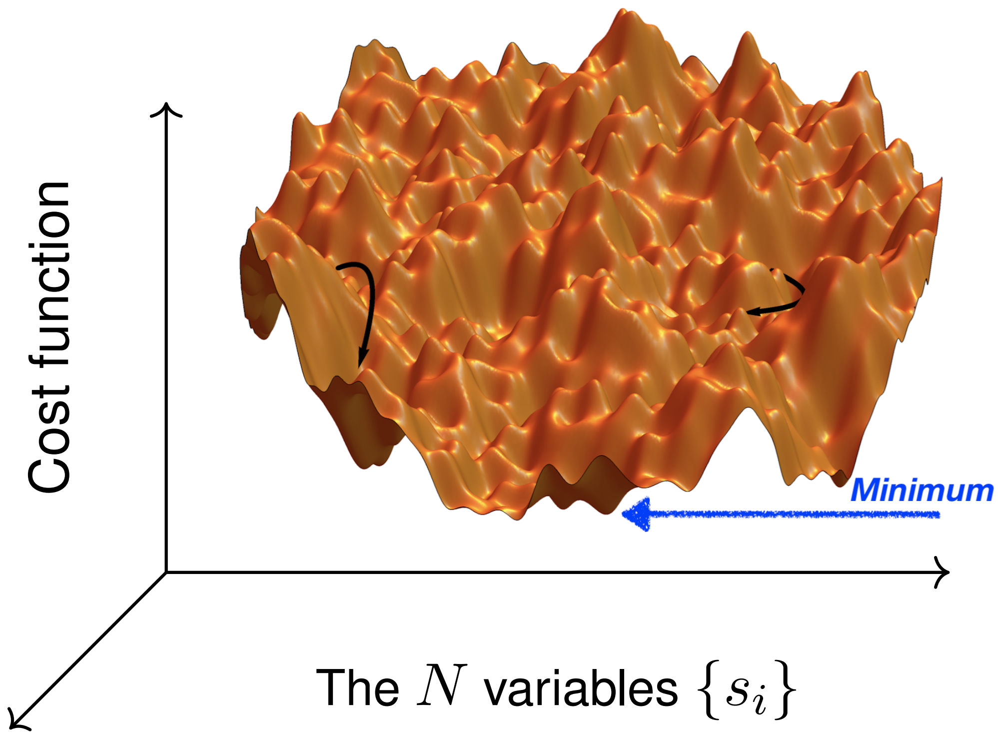


The characterization of these lanscapes is

a full field of research in math & physics

Cost function

Rugged landscape in a large dimensional space - a sketch

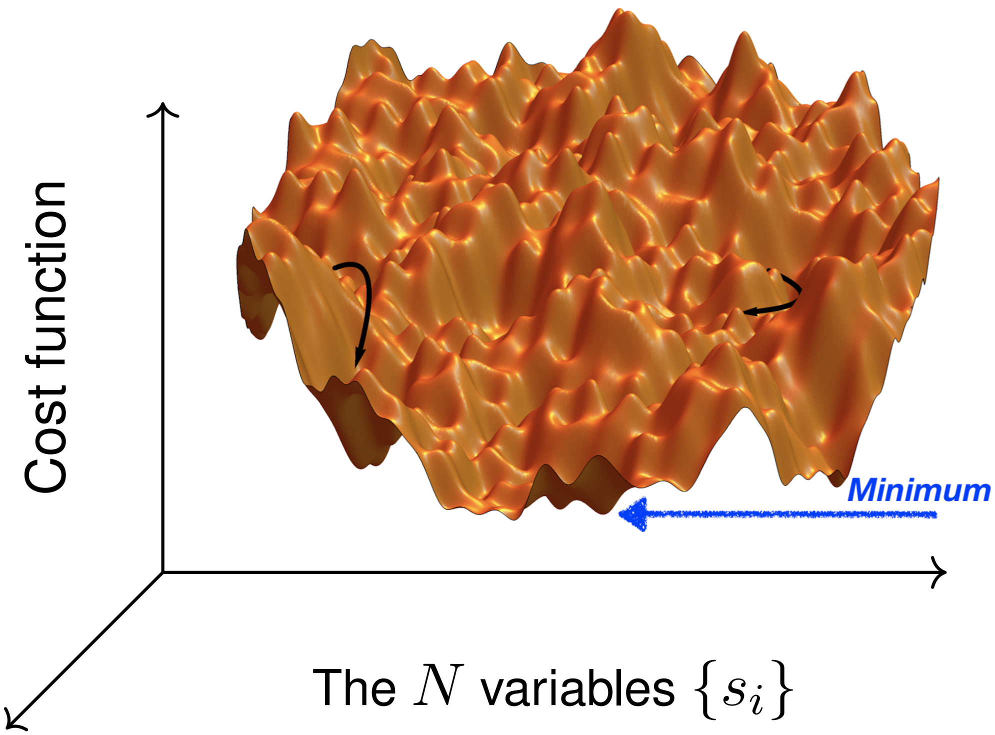


How to move on this landscape ?

Use algorithms which change the $\{s_i\}$ with some rule

Cost function

Rugged landscape in a large dimensional space - a sketch



To reach the absolute minimum is often a very hard problem

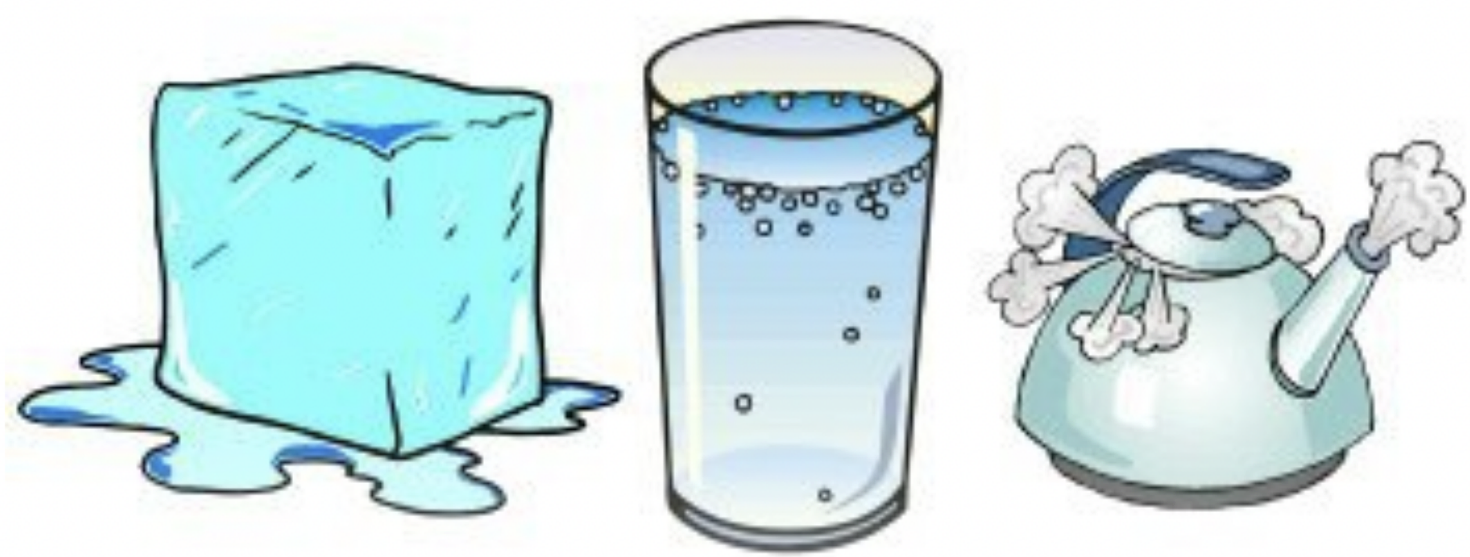
Smart algorithms ?

Let us move on to physics

Experiments, observations and **models**

States of Matter

The common ones



Solid	Liquid	Gas
ice	water	vapour

Drawing V. K. Singh

Glasses

Ancient - modern

Glasses

Peculiar physical features : neither crystals nor liquids

Relaxation time vs. inverse temperature

— Often, cooling down or pressing a liquid one makes a **glass** instead of a crystal

— **Rigid** but microscopically **disordered**

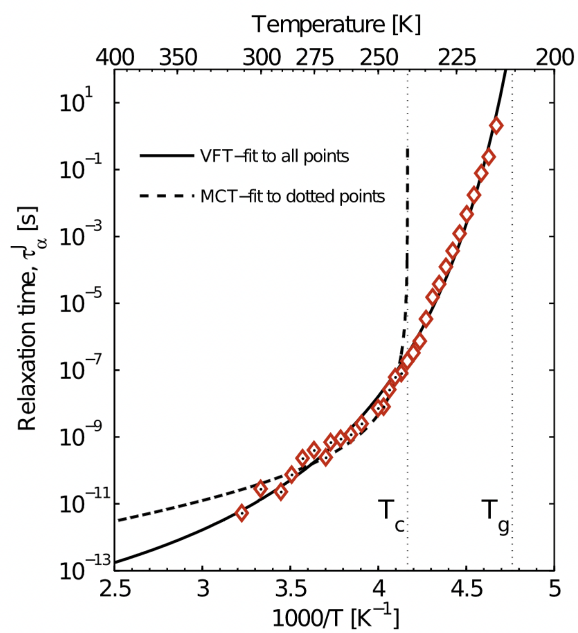
— Extremely **slow macroscopic dynamics**

relaxation time grows by orders of magnitude

under weak changes of the external conditions

— Out of equilibrium evolution

(a bit more technical)

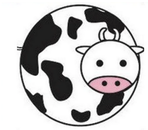


super-cooled liquid   glass

Experiments

Cost function

Another equation - the "spherical cow" model



The **standard model** of glassy behaviour

Huge conceptual jump !

$$C = \underbrace{\sum_{i \neq j \neq k \neq l}}_{\text{sum over all groups of four}} \underbrace{J_{ijkl}}_{\text{interactions}} \underbrace{s_i s_j s_k s_l}_{\text{variables}}$$

There are N variables $s_i = \pm 1$

and $N(N-1)(N-2)(N-3)/4$ predetermined couplings J_{ijkl}

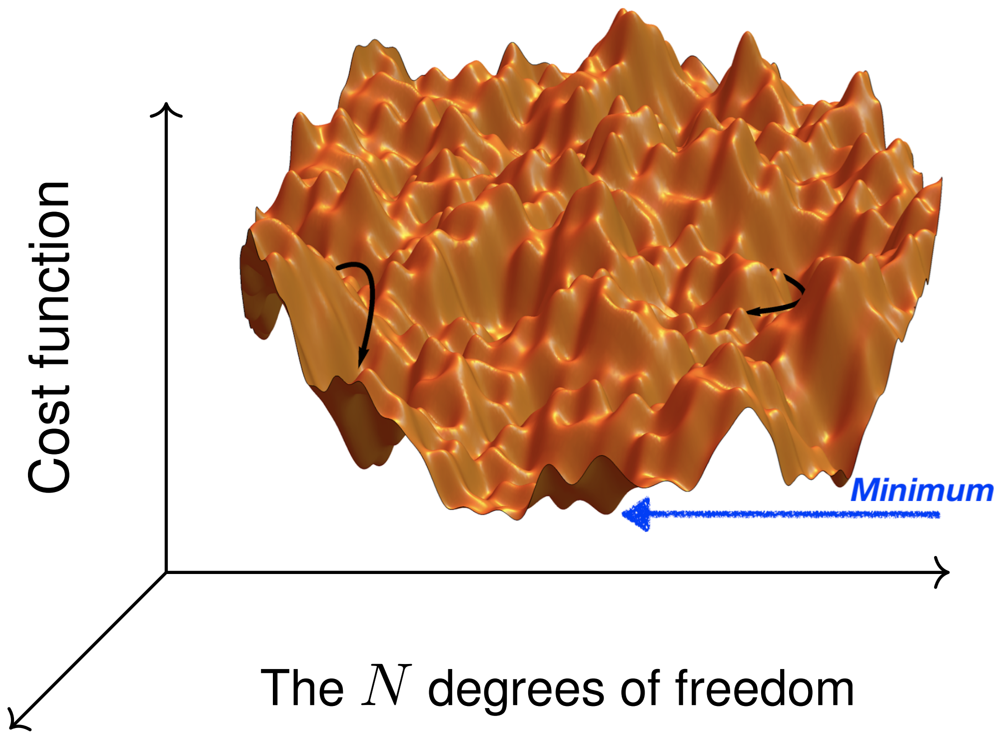
(like $J_{ijkl} = +1$ or $J_{ijkl} = -1$)

Similarities : **long relaxation times** (plot above), **thermodynamic properties**

Predictive power !

Rugged landscapes

In large dimensional spaces

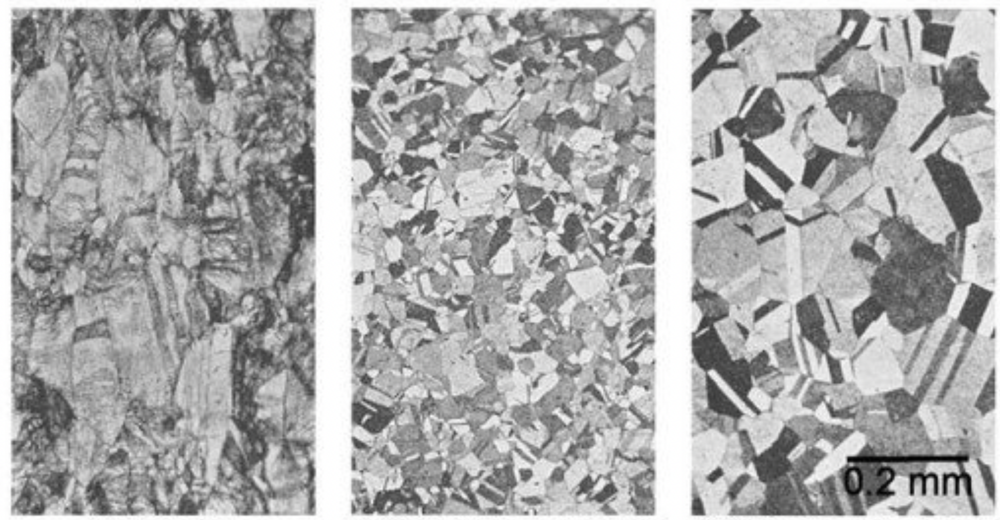


How to reach the absolute **minimum**, in the physical case the **crystal** ?

A **higher lying** region of the landscape corresponds to the **glass**

A strategy : annealing

From medieval swords to solar cells



Cold-rolled | 550 °C anneal for 1 hour | 650 °C anneal for 1 hour

ARMS ⊕ ARMOR

steel (iron with an alloy of carbon)

annealing lets the carbon move

Solar cells

Controllable crystallisation plays a crucial role in the formation of high-quality perovskites

Changing ambient conditions with a convenient protocol

to obtain the desired material properties

Annealing

Real (materials) and simulated (optimisation)

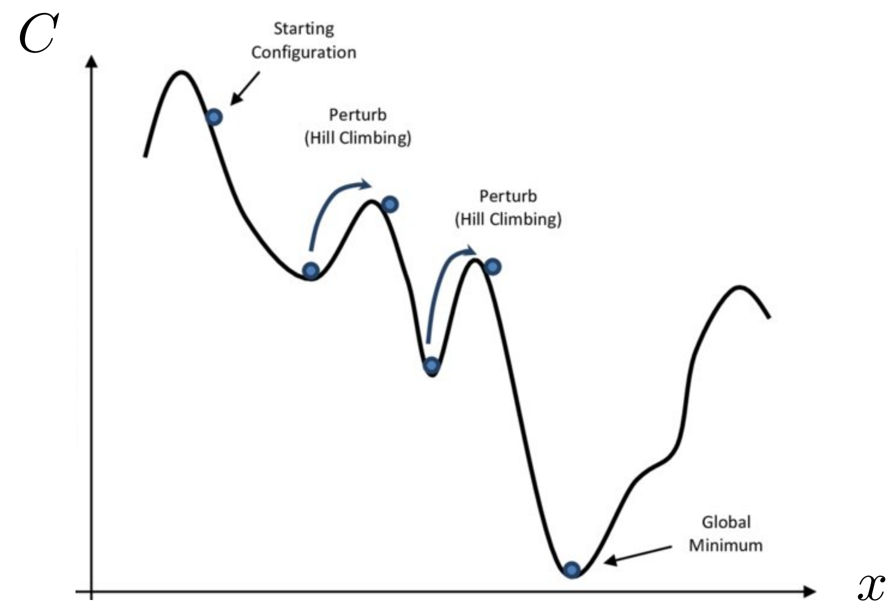


Figure from O. Ghasemalizadeh et al. 16

A physical protocol applied in the computer optimisation context

Further knowledge of the physical systems helps

in the computer science context

Black holes

Black holes

What are they ?

— A (tiny) region of spacetime where **gravity** is so strong that nothing, not even light, can escape it

— The theory of **general relativity** predicts that a sufficiently compact mass can deform spacetime to form a black hole

Einstein, Schwarzschild

— They can form through the collapse (on itself) of a big star

C. Murphy

— Can be detected indirectly, by noticing how nearby stars act differently than far away ones

Black holes

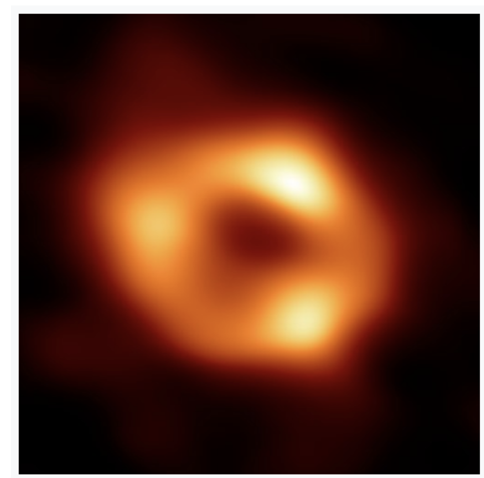
There are many nearby

Sagittarius A* is a supermassive black hole at the Galactic Center of the Milky Way

27000 light-years away from Earth

mass one million times the one of the Sun

packed within 4000 times the Earth's diameter



R. Genzel (Munich) and Andrea Ghez (Los Angeles)

Event Horizon Telescope, a world-wide network of radio observatories

Cost function

Third equation - another "spherical cow" model

A simple **quantum model** of a black hole

$$C = \underbrace{\sum_{i \neq j \neq k \neq l}}_{\text{sum over all groups of four}} \underbrace{J_{ijkl}}_{\text{interactions}} \underbrace{\psi_i \psi_j \psi_k \psi_l}_{\text{variables}}$$

There are N (Majorana $\psi_i \psi_j = -\psi_j \psi_i$) fermionic variables ψ_i

Interactions, like $J_{ijkl} = +1$ or $J_{ijkl} = -1$

The **rugged landscape** has the properties expected for a black hole, and the **thermodynamics** and **time evolution** as well

Conclusions

Connections *via* cost functions

Hard computational problems

Glasses

Black holes

In **theoretical physics**, we often use simplified models which capture the essence of a natural phenomenon. We love them for their relative mathematical manageability but also because of their predictive power, which may let us uncover unknown features of Nature.