Computational optimisation, glasses & black holes :

A rare mix with many common features

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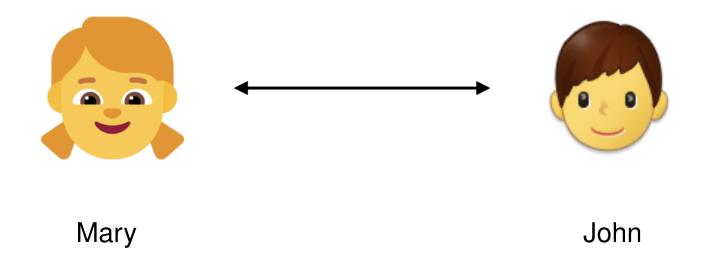
www.lpthe.jussieu.fr/~leticia/seminars

Fédération Friedel-Jacquinot, 2023

Computational optimisation

Setting

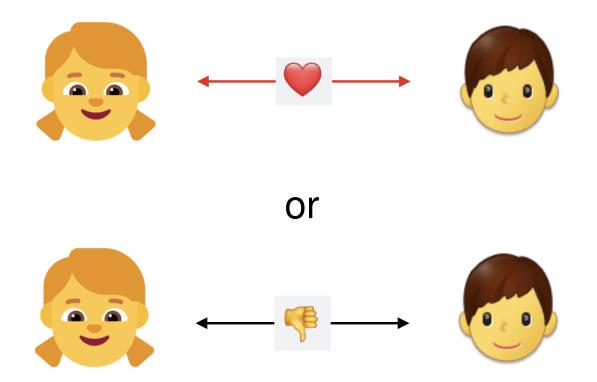
Take two individuals



They may like or dislike each other



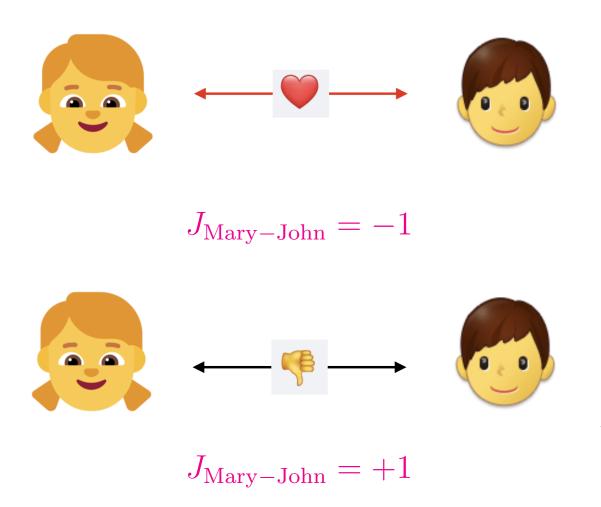
Identify their feelings towards each other



Assume they are reciprocal



Define a pairwise interaction



An easy problem

Going out for dinner in a group of three



Happy dinner

An easy problem

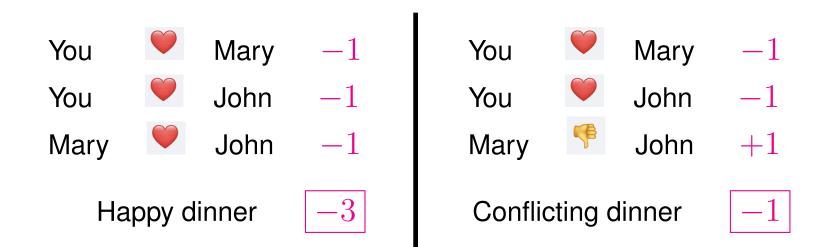
Going out for dinner: give a score



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

Easy vs. constrained

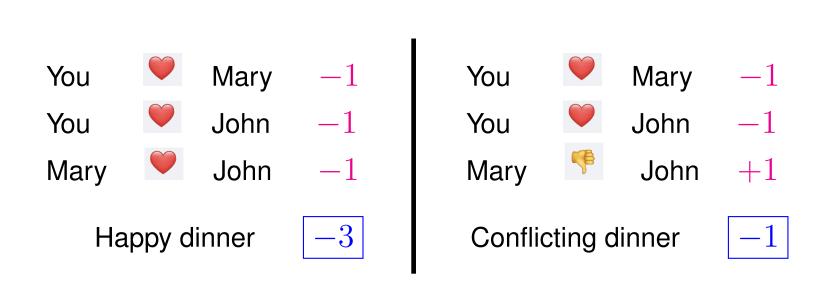
Going out for dinner in a group of three



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

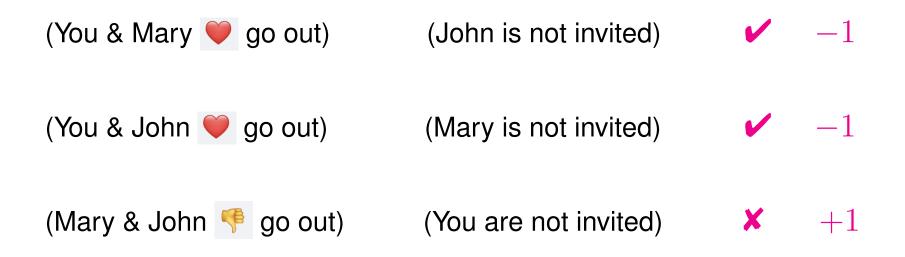


The rule is to add J = -1 for each happy pair and J = +1 for each unhappy one

The cost function takes a higher value when there is frustration

Change the proposal: split the group in two

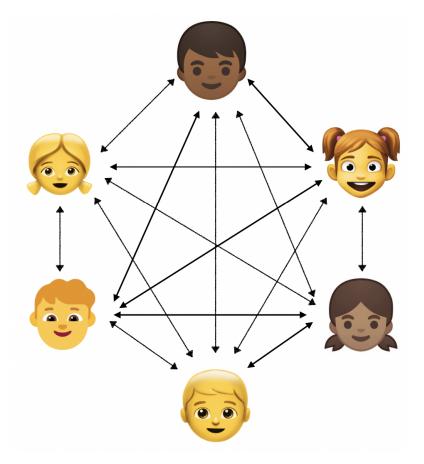
Three cases



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

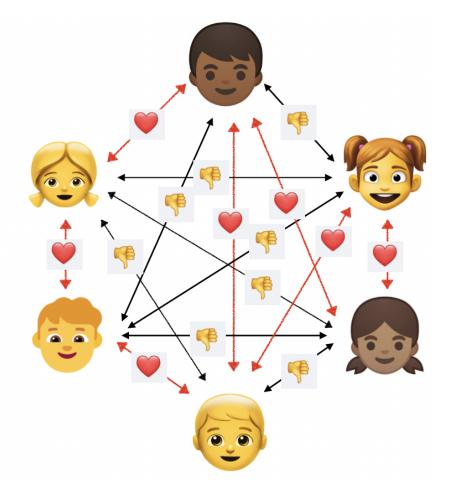
There are two **optimal** solutions which **minimise** the **cost function**

More people, many more connections



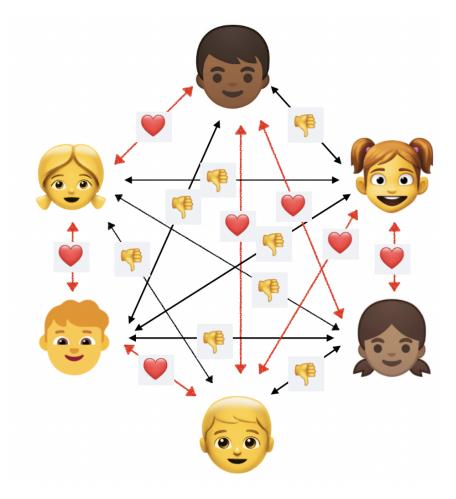
 $(N = 6 \text{ children and each has } N - 1 = 5 \text{ connections}: \frac{6 \times 5}{2} = 15 \simeq N^2/2 \text{ connections})$

More people give more possibilities & complexity increases

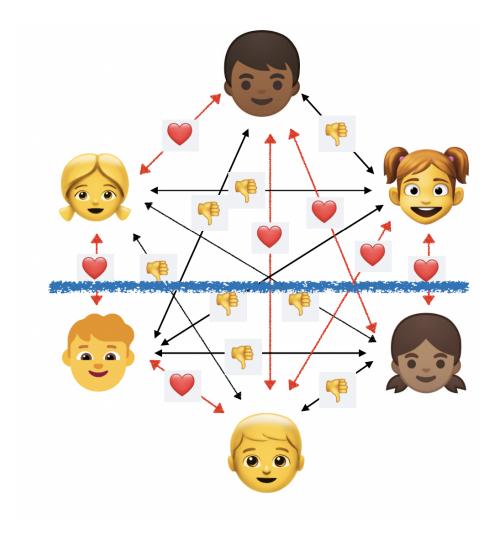


Say that, approximately, half and half love 🤎 or hate 👎 each other

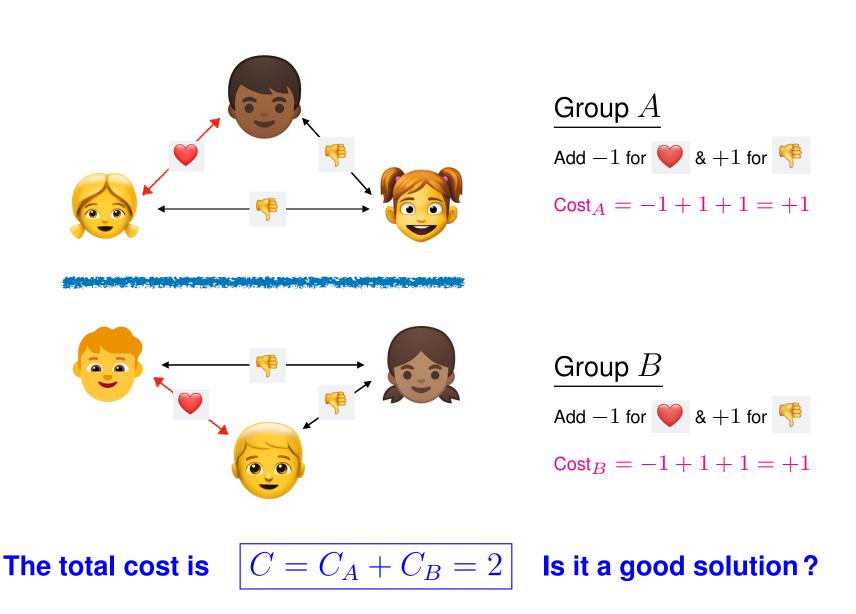
How do we split the group equally (& make two parties)?



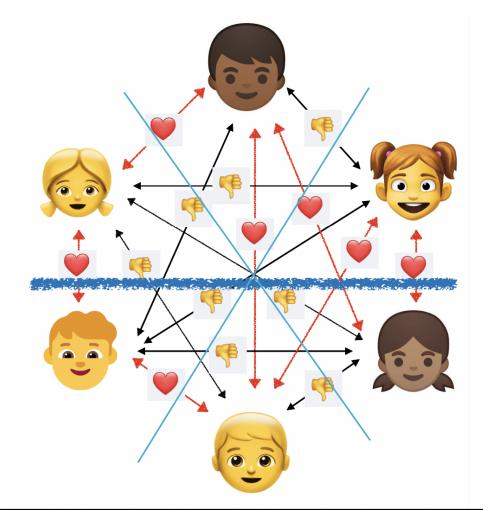
One try to split, but is it good?



Evaluate the cost function



Which is the optimal partition? A hard problem



One can try all possible cuts if there are a few persons but not if there are many!

Mathematical representation

Setting the problem in a form amenable to calculations

Its construction

In the graph partitioning - group splitting example

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

Its construction

In the graph partitioning - group splitting example

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

Each pair has a predetermined interaction

 $J_{ij} = -1$ if love \heartsuit or $J_{ij} = +1$ if hate \clubsuit between i and j

Its construction

In the graph partitioning - group splitting example

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

Each pair has a predetermined interaction

 $J_{ij} = -1$ for \heartsuit love or $J_{ij} = +1$ for \clubsuit hate

Assignment, distribution of persons

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

Its construction

In the graph partitioning - group splitting example

- $ullet \, i,j=1,\ldots,N$ label the persons
- Predetermined interactions $J_{ij} = -1$ for \mathbf{e} love or $J_{ij} = +1$ for \mathbf{e} hate
- $s_i = +1$ if i is in group A or $s_i = -1$ if i is in group B

Condition (take N even)

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

represents a sum over all i (persons) of their states given by the values of the s_i

Its construction

In the graph partitioning - group splitting example

- $i, j = 1, \ldots, N$ label the persons.
- Predetermined $J_{ij} = -1$ for \heartsuit love or $J_{ij} = 1$ for \clubsuit hate feelings
- $s_i = 1$ 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

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

is minimised

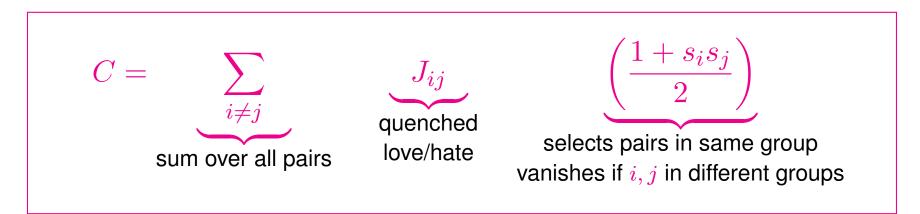
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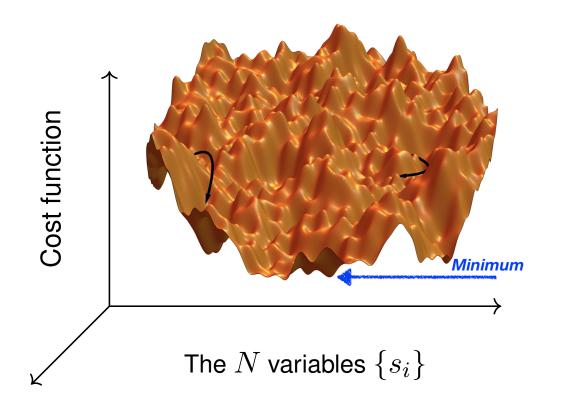
find the assignment of all the s_i so that they add up to zero $(\sum_{i=1}^N s_i = 0)$ & the

Cost function is minimised



Rugged landscape in a large dimensional space

a sketch for a given realisation of the love/hate couplings J_{ij}



How to reach the absolute minimum?

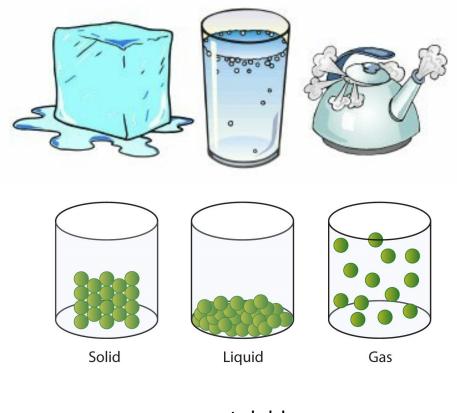
Smart algorithms?

Let us move on to physics

Experiments, observations and **models**

States of Matter

The common ones



rigid

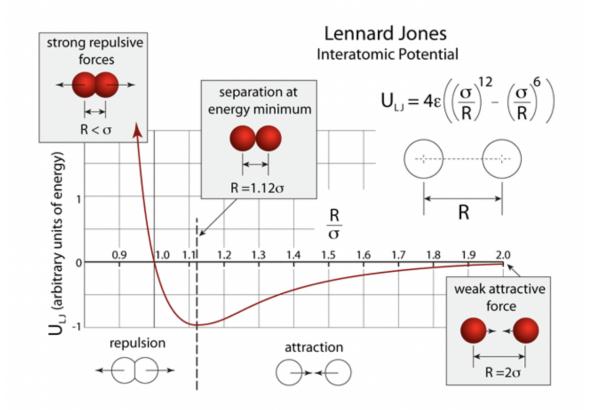
fixed shape hard to compress does not flow ordered not rigid no fixed shape hard to compress flows disordered

not rigid no fixed shape easy to compress flows disordered

Matter

Models for the particle interactions

Typically, repulsive or attractive depending on distance



How does an ensemble of many such interacting particles spatially arrange? New "glass phase" under certain conditions

Ancient - modern



Peculiar physical features

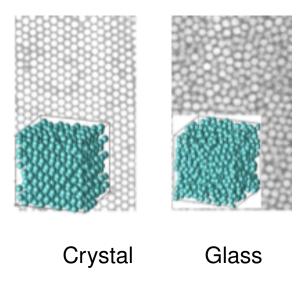
Structure

- Rigid but microscopically disordered

(very different from a crystal)

Extremely slow macroscopic dynamics
 relaxation time grows by orders of magnitude
 under weak changes of the external conditions

Out of equilibrium evolution
 (no Gibbs-Boltzmann measure reached)



Experiments

Peculiar physical features

Relaxation time vs. 1/temperature

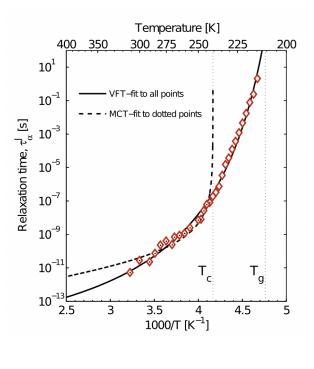
Rigid but microscopically disordered

(very different from a crystal)

Extremely slow macroscopic dynamics

relaxation time grows by orders of magnitude under weak changes of the external conditions

— Out of equilibrium evolution (no Gibbs-Boltzmann measure reached)



super-cooled liquid glass

Experiments

Peculiar physical features

Self intermediate scattering fct vs. time-delay

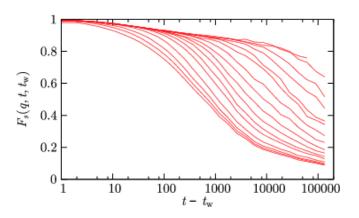
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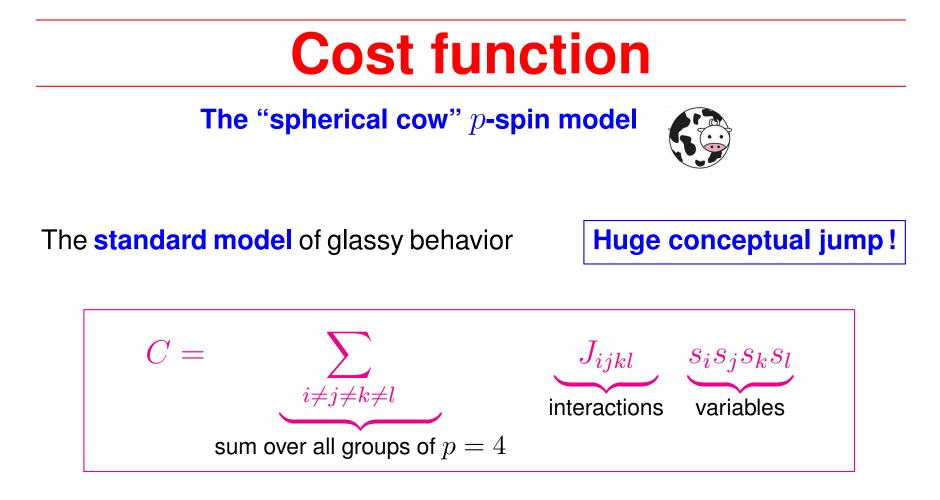
Out of equilibrium evolution

(no Gibbs-Boltzmann measure reached)



Aging in Lennard-Jones mixtures

Simulations



There are $i, j, k, l = 1, \ldots, N$ variables

and N(N-1)(N-2)(N-3)/4 predetermined couplings J_{ijkl} from a p.d.f.

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

Phenomenology: thermodynamics, long relaxation times, rugged landscapes

p-spin models

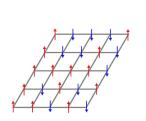
Capture many physical systems

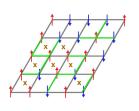


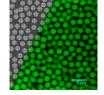
- Forgot particles and used binary $s_i=\pm 1\,$ or spherical $\sum\limits_{i=1}^N s_i^2=N$ variables
- $\ensuremath{\, \bullet \,}$ Instead of finite d real space placed the spins on a complete (hyper-)graph

Interactions Spins System Model

Two-body Spherical FMs Curie-Weiss **Two-body Ising** Spin glass SK model $p \geq 3$ -body Ising or spherical (Fragile) Glasses p-spin







Some methods

for systems with quenched randomness

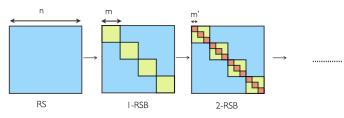
Edwards-Anderson (75) dynamic order parameter, replica trick

Thouless-Anderson-Palmer (77) extension of the familiar free-energy

$$f(m) = \frac{Jz}{2}m^2 - \ln[2\cosh(\beta Jzm + \beta m)]$$
$$m = \tanh(\beta Jzm + \beta h)$$

to an N order parameter $\{m_i\}$ dependent $f_J(\{m_i\})$: rugged landscape

Parisi : Replica Symmetry Breaking (79-83)



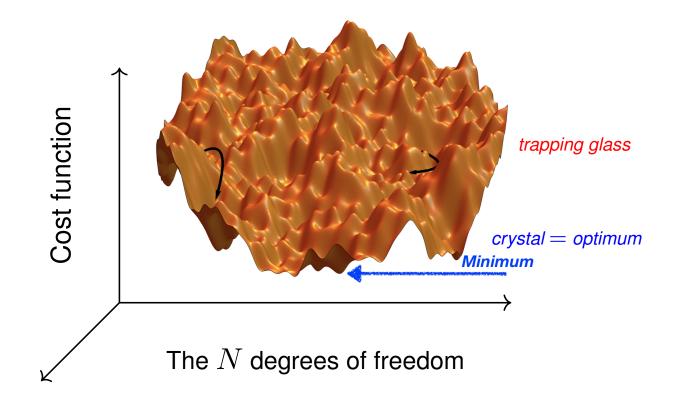


the equilibrium properties, further information about the "state" organization, etc.

On the plateau Franz, Ros, Rosso (LPTMS), Foini, Urbani (IPhT)

Rugged landscapes

In large dimensional spaces



How to reach the absolute minimum, in the particles' case the crystal? Other regions of the landscape correspond to the glass

Rugged landscapes

In large dimensional spaces

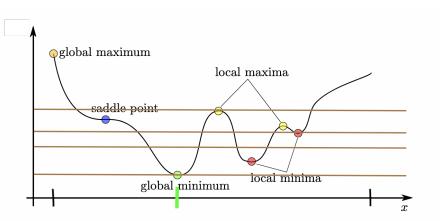
Hard to think in large dimensional spaces: not much intuition

In the hard optimization problems or glassy ones

an exponentially large number of minima/maxima/saddle-points

 $\# = e^{N\Sigma}$

at \neq heights in the landscape



 Σ is called **configurational entropy** or **complexity**

Much work on the analysis of these landscapes, first by theoretical physicists, more recently by mathematicians Familiar strategies to surf down the landscape

Annealing

From medieval swords to everyday life



ARMS ⊕ ARMORsteel (iron with an alloy of carbon)
annealing lets the carbon move

Granular matter

shaking coffee jar to compact the grains and let them occupy less space

Changing ambient conditions with a convenient protocol

Annealing

Real and simulated

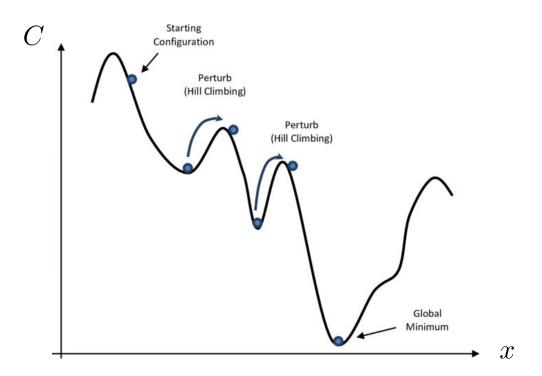


Figure from O. Ghasemalizadeh et al. 16

A physical protocol applied in the computer optimization context

Modern strategies

Use knowledge about the landscape

to devise smarter algorithms

Extensions of simulated annealing

Replica simulating annealing Baldassi et al. (16), Angelini & Ricci-Tersenghi (22)

Message passing algorithms

Belief propagation Pearl (82), Kabashima & Saad (90s), Yedidia (01)

Survey propagation Mézard, Parisi, Zecchina (02)

Much more to be said, if interested, contact the experts

Relaxation in the glass Global observables

Two-time correlations and linear responses

Two-time dependencies

Self-correlation and linear response

The two-time self correlation and integrated linear response

$$C(t,t_w) \equiv \frac{1}{N} \sum_{i} \left[\langle s_i(t)s_i(t_w) \rangle \right]$$

$$\chi(t,t_w) \equiv \frac{1}{N} \sum_{i} \int_{t_w}^t dt' \ R(t,t') = \frac{1}{N} \sum_{i} \int_{t_w}^t dt' \ \left[\frac{\delta \langle s_i(t) \rangle_h}{\delta h_i(t')} \right|_{h=0} \right]$$

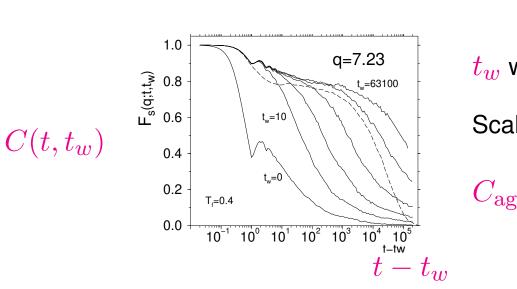
Extend the notion of order parameter

They are not related by FDT out of equilibriumMagnetic notation but generalThe averages are thermal (and over initial conditions) $\langle \dots \rangle$ and over quenched randomness $[\dots]$ (if present)

 t_w waiting-time and t measuring time

Two-time self-correlation

In glassy systems



 $T < T_q$

Lennard-Jones mixtures

 t_w waiting time

Scaling below the envelope

$$C_{\rm ag}(t, t_w) \sim f_{\rm ag}\left(\frac{\mathcal{R}(t)}{\mathcal{R}(t_w)}\right)$$

Aging: older systems relax more slowly than younger ones

Dynamic equations

On the correlation and linear response for Langevin dynamics

In the $N \to \infty$ limit exact causal Schwinger-Dyson (DMFT) equations

$$(\gamma \partial_t - \mathbf{z_t})C(t, t_w) = \int dt' \left[\Sigma(t, t')C(t', t_w) + D(t, t')R(t_w, t') \right] + 2\gamma k_B T R(t_w, t) (\gamma \partial_t - \mathbf{z_t})R(t, t_w) = \int dt' \Sigma(t, t')R(t', t_w) + \delta(t - t_w)$$

where Σ and D are the self-energy and vertex. For the p spin models

 $D(t,t') = \frac{p}{2} C^{p-1}(t,t') \qquad \Sigma(t,t') = \frac{p(p-1)}{2} C^{p-2}(t,t') R(t,t')$

The Lagrange multiplier z_t is fixed by C(t, t) = 1. Random initial conditions.

(Average over randomness already taken; later, interest in noise-induced fluctuations)

Predictions

Aging and reparametrization invariance

Aging is derived analytically
$$C_{ag}(t, t_w) \sim f_{ag}\left(\frac{\mathcal{R}(t)}{\mathcal{R}(t_w)}\right)$$
 with $\frac{\mathcal{R}(t)}{\mathcal{R}(t_w)} = \mathcal{O}(1)$
Slow relaxation $\partial_t C_{ag}(t, t_w) \propto \frac{\dot{\mathcal{R}}(t)}{\mathcal{R}(t)} \xrightarrow[t \to \infty]{} 0 \implies \partial_t C_{ag}(t, t_w) \ll C_{ag}(t, t_w)$

Dropping the time-derivatives, approximate eqs. for the slow relaxation, i.e.

 $C_{
m ag}$ (below the envelope) and the corresponding $R_{
m ag}$

Invariant under time-reparametizations

$$t \to h_t \equiv h(t) \qquad \begin{cases} C_{\rm ag}(t, t_w) \to C_{\rm ag}(h_t, h_{t_w}) \\ R_{\rm ag}(t, t_w) \to \frac{dh_{t_w}}{dt_w} R_{\rm ag}(h_t, h_{t_w}) \end{cases}$$

with h_t positive and monotonic

Turn it useful

Reparametrization invariance \Rightarrow **fluctuations**

Noted by

classical Sompolinsky & Zippelius (83), Ginzburg (86), Ioffe (88), LFC & Kuchan (93), Franz & Mézard (94) quantum Castillo, Chamon, LFC & Kennett (02)

Used to characterize fluctuations in real space beyond mean-field

Castillo, Chamon, Charbonneau, LFC, Iguain, Kennett, Sellitto, Reichman (02-07)

Quote from Chamon & LFC 07 review

values of the two laboratory times. The fact that the effective dynamical action becomes invariant under global time reparametrizations, $t \to h(t)$, everywhere in the sample means that the action weights the fluctuations of the proper ages, $C(\vec{r}; t_1, t_2)$, directly, and the times t_1 and t_2 in the action are just integrated over as dummy variables. To draw an analogy, in theories of quantum gravity the space-time variables $X_{\mu}(\tau, \sigma)$ are the proper variables and the action is invariant under conformal transformations of the world-sheet parameters τ and σ .

relation to gravity?

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-Oppenheimer

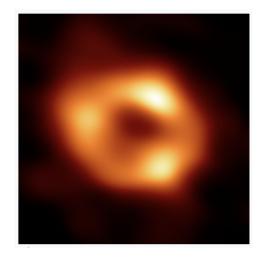
 Can be detected indirectly, by noticing how nearby stars act differently than far away ones

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

Gravity & quantum field theory

Holography - Duality

Quantum gravity (compactified string theories)

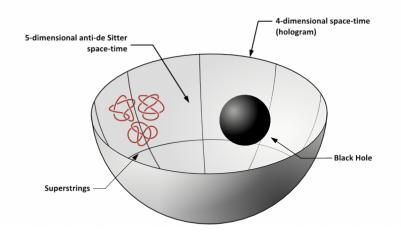
in a d+1 dimensional space with Anti-deSitter geometry

AdS

Quantum Field Theory with conformal symmetry

on the d dim. boundary with local Minkowski metric

CFT



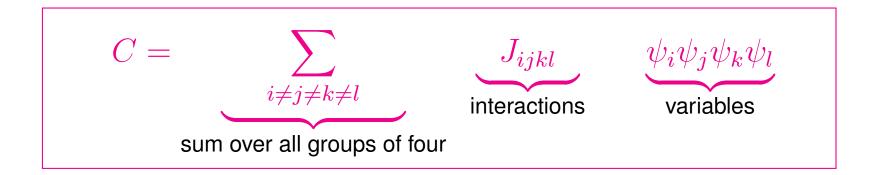
Proposed by Maldacena (97)

Applications in condensed matter Sachdev

Cost function



Based on **holography**, a simple d = 0 quantum model of a black hole



There are i, j, k, l = 1, ..., N Majorana fermions, $\psi_i^{\dagger} = \psi_i$ and $\{\psi_i, \psi_j\} = 0$ Random interactions J_{ijkl} with $[J_{ijkl}] = 0$ and $[J_{ijkl}^2] = 4!J^2/N^3$

The entropy $S(T) \xrightarrow{T \to 0} a + bT$ & time evolution similar to black hole ones

Dynamics

The SY Kitaev - another "spherical cow" - model



$$\frac{\partial q_d(\tau,\tau')}{\partial \tau} = \delta(\tau-\tau') + \int_0^{\beta\hbar} d\tau'' \,\Sigma(\tau,\tau'') q_d(\tau'',\tau')$$

with τ the imaginary time, $q_d(\tau, \tau') \equiv \frac{1}{N} \sum_{i=1}^N \mathcal{T}[\langle \psi_i(\tau) \psi_i(\tau') \rangle]$ the correlation and $\Sigma(\tau, \tau') \equiv J^2 q_d(\tau, \tau')^3$ the self-energy

Slow dynamics for long $\tau - \tau' \implies$ drop the time-derivative and then

time reparametrization invariance under

$$\tau \mapsto h(\tau) \qquad q_d(\tau, \tau') \mapsto [h(\tau)h(\tau')]^{1/4} q_d(h(\tau), h(\tau'))$$

and, by holography, invariance under diffeomorphisms of general relativity



Connections *via* **cost functions & dynamics**

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.

Glassy mean-field models

Classical p-spin spherical

Potential energy

$$\mathcal{V} = -\sum_{i_1 \neq \dots \neq i_p} J_{i_1 \dots i_p} \, s_{i_1} \dots \, s_{i_p} \qquad p \text{ integer}$$

quenched random couplings $J_{i_1...i_p}$ drawn from a Gaussian $P[\{J_{i_1...i_p}\}]$

(over-damped) Langevin dynamics for continuous spins $s_i \in \mathbb{R}$ coupled to a white bath $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = 2\gamma k_B T \delta(t - t')$

$$\gamma \frac{ds_i}{dt} = -\frac{\delta \mathcal{V}}{\delta s_i} + z_t s_i + \xi_i$$

 z_t is a Lagrange multiplier that fixes the spherical constraint $\sum\limits_{i=1}^N s_i^2 = N$

 $p=2 \text{ mean-field } \mbox{domain growth} \\ p\geq 3 \mbox{ RFOT modelling of fragile glasses} \\$