Statistical Physics 2: Disordered Systems and Interdisciplinary Applications 12.02.2021

Application of stat mech of disordered systems to computer science

I Computer science problems

1. Decision problems : yes/no answer

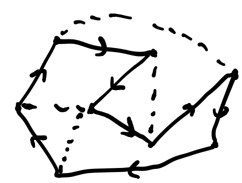
Examples:

- Hamiltonian circuit (or cycle)

  $G = (V, E)$ Is there a Hamiltonian circuit?

  a closed path that visits each vertex exactly once

- Traveling salesman problem (TSP)



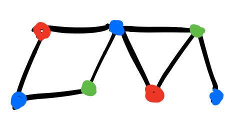
  G weighted w_{ij}

  Is there a Hamiltonian cycle $\sum_{k=1}^{N} w_{i_k i_{k+1}} \leq W$?

  Applications in planning, logistics, ...

- Coloring problem (e.g. for maps)

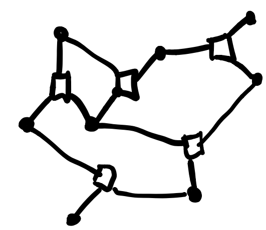
  G Is there an assignment of q colors to vertices such that no edge is monochromatic?



  $\{\sigma_1 \cdots \sigma_N\} \in \{1 \cdots q\}^N$

  $\sigma_i \neq \sigma_j$ for $\forall \langle ij \rangle \in E$

- K-XORSAT problem



G K-hypergraph

M edges $a = 1 \dots M$

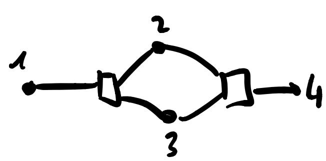
$\partial a = \{ i_1^a \dots i_K^a \}$

$x_i \in \{0,1\}$ and $y_a \in \{0,1\}$

Is there a solution to the set of linear eqs

$$x_{i_1^a} + x_{i_2^a} + \dots + x_{i_K^a} = y_a \quad \text{mod } 2$$

$$\begin{cases} 1+0 = 0+1 = 1 \\ 0+0 = 1+1 = 0 \end{cases} \quad \text{exclusive OR} \quad \text{XOR}$$



$$x_1 + x_2 + x_3 = 0$$
$$x_2 + x_3 + x_4 = 1$$

Define $\sigma_i = (-1)^{x_i} \in \{\pm 1\}$

$J_a = (-1)^{y_a} \in \{\pm 1\}$ $\qquad \prod_{i \in \partial a} \sigma_i = J_a$

- K-SAT problem

Same as K-XORSAT but OR instead of XOR

$$x_{i_1^a} \vee \overline{x}_{i_2^a} \vee \cdots \vee \overline{x}_{i_K^a} \qquad a = 1 \dots M$$

$$\sigma_{i_1^a} = J_1^a \vee \sigma_{i_2^a} = J_2^a \vee \dots \vee \sigma_{i_K^a} = J_K^a$$

- Perceptron problem (continuous variables)

Patterns $\vec{\xi}_a \in \mathbb{R}^N$

Is there $\vec{x} \in \mathbb{R}^N$ s.t. $|\vec{x}|^2 = N$ and $\vec{\xi}^a \cdot \vec{x} \geq \sigma \sqrt{N}$?

2. Complexity classes for decision problems

"quenched disorder" aka "instance" : G, J

"variables" : the cycle, $\{x_i\} \to \{\sigma_i\}$

A given instance (formula) is SAT if answer is yes
UNSAT " no

"Size" of the instance : N, number of vertices

$\boxed{\text{NP class}}$ ("easy to check")

A problem is in NP if given a solution, you can check it in poly(N) time

All example above are in NP

Find a solution by "brute force" : time 2^N, q^N, $N!$

<u>Question</u>: is there a poly(N) algorithm to solve the problem (yes/no) ?

$\boxed{\text{P class}}$ (2-COL, 2-SAT, K-XORSAT)

There are algorithms that give the solution in poly(N) time <u>for all instances</u>

Ex: 2-COL : assign color 1 to a vertex, color 2 to neighbors,
K-XORSAT : Gaussian elimination

But: K-SAT $_{K \geq 3}$, q-COL $_{q \geq 3}$, TSP

For the moment no poly(N) algorithm for all instances

A NP problem can become P

$\boxed{\text{NP-complete problems}}$ "Hardest problems in NP"

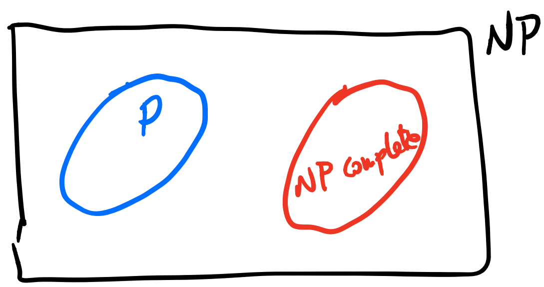
Problem A is NP-complete if $A \in NP$ and

for $\forall B \in NP$ an instance of B of size N can be mapped in poly(N) time into an instance of A of size $N' \sim$ poly(N)

If $A \in P \Rightarrow NP = P$

It is believed that $P \neq NP$, i.e. NP-complete problems cannot be solved in poly(N) time

1 M\$ to prove or disprove (millennium prize problems)



K-SAT $_{K \geq 3}$, q-GL $_{q \geq 3}$, TSP are all NP-complete

Other complexity classes for:

- optimization problems : find the best W for TSP
  find the ground state of the SK model
- counting problems : how many colorings of a G ?

II. Stat mech approach to constraint satisfaction pbs

1. the partition function

q-COL, K-SAT, K-XORSAT : configurations $\underline{\sigma} = \{\sigma_1 \dots \sigma_N\}$

$$H[\underline{\sigma} ; G, J] = \sum_{a=1}^{M} \mathbb{1}[\underline{\sigma} \text{ violates constraint } a]$$
$$= (\# \text{ of violated constraints})$$

Ex. COL: no J, $a = \langle ij \rangle \in E$, $H[\underline{\sigma}, G] = \sum_{\langle ij \rangle \in E} \delta_{\sigma_i \sigma_j}$.
(AF Potts model)

SAT instance $\Leftrightarrow \min_{\underline{\sigma}} H[\underline{\sigma} ; G, J] = 0$

One way : stat mech at $T=0$

$$Z(\beta ; G, J) = \sum_{\underline{\sigma}} e^{-\beta H[\underline{\sigma} ; G, J]} \xrightarrow[\beta \to \infty]{} \mathcal{N}_{sol.}(G,J)$$

Usual situation for disordered systems

$\underline{\sigma}$ thermal average ; $\{G, J\}$ disorder average

2. Random instances

Computer Science complexity classes are defined in the "worst case scenario" over $\{G, J\}$

Paradox in the 80s

- many problems proven to be NP complete
- simple algorithms could solve many instances

Question: how do we construct difficult instances?

Idea: random instances

- benchmarks
- practical way to construct difficult instances
- sometimes useful for applications

Examples:

q-COL of Erdös-Rényi graph $\longrightarrow$ AF Potts model on ER graph

N vertices, $M = \alpha N$ edges

K-XORSAT
K-SAT

on a random ER hypergraph

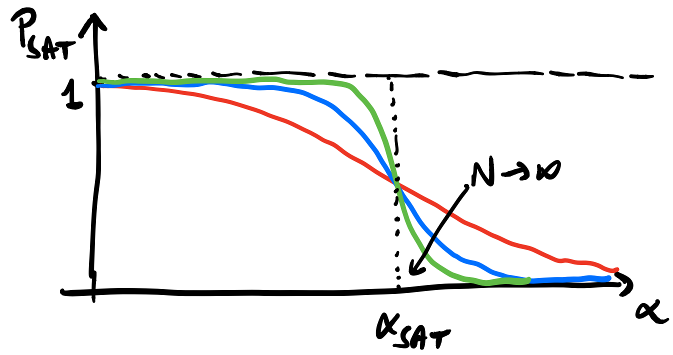
N vertices
$M = \alpha N$ hyperedges
$J = \pm 1$ at random

Control parameters: α, $\overset{q}{K}$, $T \to 0$, $N \to \infty$

Fix q, k - vary α, N

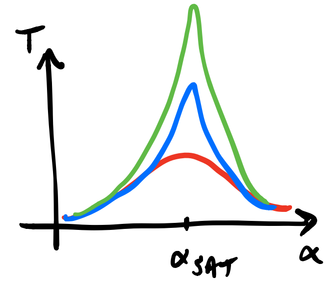
$$P_{SAT}(\alpha, N) = \{\text{fraction of SAT instances}\}$$

Numerical results: (3-SAT)



$$P_{SAT}(\alpha, N) \to \begin{cases} 1 & \alpha < \alpha_{SAT} \\ 0 & \alpha > \alpha_{SAT} \end{cases}$$

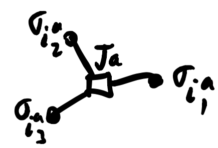
A phase transition!



Hard instances found around α_{SAT}

In the tutorial: discuss bounds on α_{SAT} for K-XORSAT

3. Spin glass phase diagram.



K- XORSAT

$$H[\underline{\sigma}; G, J] = \sum_{a=1}^{M} \frac{1 - J_a \sigma_{i_1^a} \sigma_{i_2^a} \cdots \sigma_{i_K^a}}{2}$$

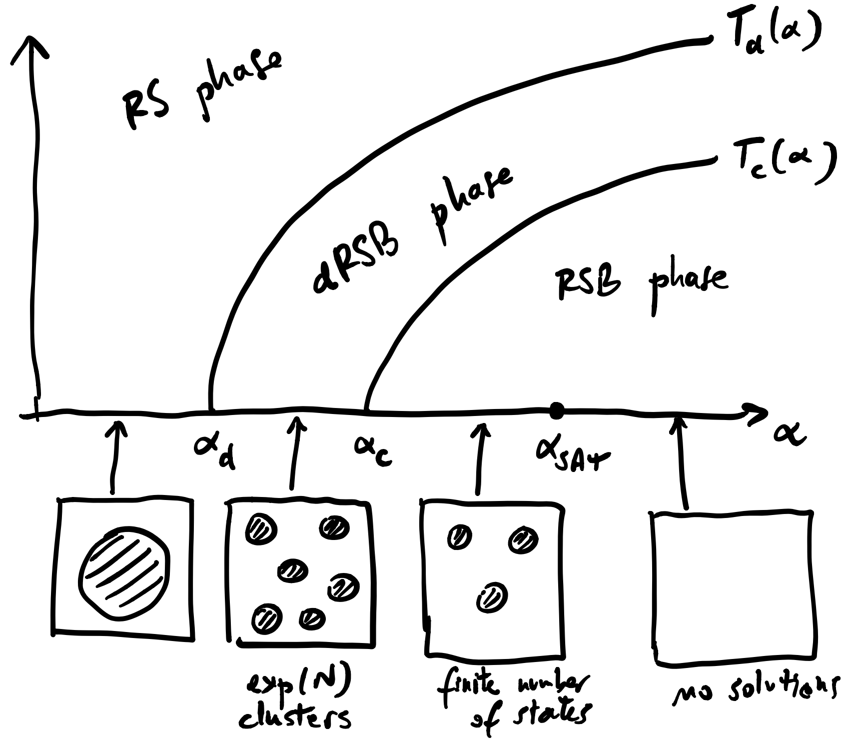
This is the pspin!
- on a ER hypergraph
- $J = \pm 1$ instead of Gaussians
- $p = K$ (note the interest of $p \geq 3$)

but $\alpha \to \infty$ (after $N \to \infty$) equivalent to fully connected

(and Gaussian equivalent to ± 1)

In $N \to \infty$ for fixed $K \ (=p)$: (α, T)

Phase diagram:



Phase space
Σ , 2^N

Glassy phase $\Rightarrow$ slow dynamics $\Rightarrow$ algorithmic difficulty

Many results obtained via spin glass techniques
Many of them have been proven rigorously

Active and interdisciplinary field
(Computer science, math, stat phys, machine learning...)

4. Conclusions

- Main message: quenched disorder
  two kind of averages
  self averaging

- Spin glasses useless materials but "prototypes" of complex systems

  Techiques have broad applicability

- Replica method a bit mysterious but now is quite well understood - rigorous proofs

- Importance of dynamics