## The Phase Transitions in the Random Coloring Problem



#### Lenka Zdeborová

In collaboration with: Florent Krzakala (Paris, ESPCI) Guilhem Semerjian (Paris, ENS) Andrea Montanari (Standford University) Federico Ricci-Tersenghi (Rome, La Sapienza)

#### Outline

Part I (1-11): Introduction, Model definition, Motivation from different perspectives; Part II (12-20): Cavity Method: basic ideas (RS and 1RSB); **Part III (21-25):** Zoology of the phase transitions in random coloring; Part IV (26-27): What did we learned, what can we do more?

## Definition of graph coloring





- State: each node has a color
- Rule (energy cost): neighbors have different colors



## Less trivial example



## How difficult is to color a graph?

#### Planar graphs:

- 10 minutes by hand for the CZ regions map ...
- Proof of 4-colorability: Appel-Haken (1976) ... probably never entirely he
ked.
- New proof: Robertson, Sanders, Seymour, Thomas  $(1994)$ ,  $N^2$  algorithm follows.
- Checking 3-colorability for planar graphs is NP-complete, Dailey (1980)

General graphs: given a graph  $G(V, E)$ ,  $|V| = N$ , and number of colors q

• Is it possible to color the graph? NP-complete

## What does it mean NP-complete?

- NP problem: If you give me a solution, I can check it in polynomial time (polynomial in size of the graph)
- P problem: I can find solution in polynomial time for every instance of the problem (for every possible graph)
- NP-complete problem (Cook 1971): If this problem would have a polynomial time solution, all the NP problems do!

The "million" problem:  $P=NP?$ Is there <sup>a</sup> polynomial algorithm for any of the NPomplete problems?

TOP 3: K-satisability, oloring, traveling salesman

#### Worst versus average

Erdös-Rényi random graphs  $G(N, p)$ : p probability that two vertexes are connected. Average degree  $\alpha = p(N - 1)$ .

What is the relevant (nontrivial) value of  $\alpha$ ?

First moment argument:  $\langle \mathcal{N} \rangle \geq \text{Prob}(\mathcal{N} > 0).$ 

$$
\langle \mathcal{N} \rangle = q^N \left( 1 - \frac{1}{q} \right)^{pN(N-1)/2} = \exp \left[ N \left( \log q + \frac{p(N-1)}{2} \log \frac{q-1}{q} \right) \right]
$$

The limit of large graphs  $N \to \infty$ ; interesting region

$$
1 < \alpha < \frac{2\log q}{\log q - \log (q - 1)} =_{q=3} 5.42.
$$

## The COL/UNCOL transition



In  $N \to \infty$  the transition is sharp. Discontinuous even in entropy.

Idea of phase transitions in purely mathematical problems - back to 1961, Erdös-Rényi – giant component (percolation) in random graphs.

## Where the Really Hard Problems are?

Cheeseman, Kanefsky, Taylor (1991); Computational ost of the Davis-Putnam bran
h and bound algorithm

We want to understand independently of any algorithm!



To know where the hard problems are is useful

- to find them (to test algorithms)
- to avoid them in the real world appli
ations
- to design new algorithms (survey propagation)

## Properties of random graphs

- Erdös-Rényi random graph ensemble: each edge present with probability  $p = \alpha/N$ . For  $N \to \infty$ ,  $\alpha$  fixed, the degree distribution is Poissonian  $p_k = e^{-\alpha} \frac{\alpha^k}{k!}$
- Regular random graphs: fixed degree  $r$ . Special simplification of the cavity equations.
- Both: loops length is or order  $\log N$  locally tree-like structure!

## Statistical physics formulation

Hamiltonian (energy function) of antiferromagnetic Potts model<br>  $\mathcal{H} = \sum \delta(s_i, s_j)$ 

$$
\mathcal{H} = \sum_{(i,j) \in E} \delta(s_i, s_j)
$$

Graph: quen
hed disorder. Average free energy

$$
\langle \log Z \rangle = -\beta F(\beta) = -\beta E + S(E)
$$

We want to compute average (over graphs) ground state energy

$$
E_{\rm gs}=\lim_{\beta\to\infty}\frac{\partial(\beta F)}{\partial\beta}
$$

If  $E_{\rm gs}$  also average ground state entropy

$$
S_{\rm gs} = -\lim_{\beta \to \infty} (\beta F)
$$

## Bethe approximation

- Approximation for lattice models, equivalent to mean field theory.
- Exact for models on random graphs, at least in presence of one or only few <sup>p</sup>hases (e.g. ferromagnet)

# Cavity method

Formulation of the Bethe approximation, whi
h is generalizable to glassy systems (many <sup>p</sup>hases, pure states).

Developed by Mézard, Parisi (1999).



Define  $\psi_{s_i}^{i \to j}$  as a probability that node *i* takes color  $s_i$  when edge (constraint)  $(ij)$  is erased from the graph. Write recursive equations for these probabilities

$$
\psi_{s_i}^{i \to j} = \frac{1}{Z^{i \to j}} \prod_{k_i nV(i) - j} \sum_{s_k} e^{-\beta \delta_{s_i s_j}} \psi_{s_k}^{k \to i}
$$

$$
= \frac{1}{Z^{i \to j}} \prod_{k_i nV(i) - j} [1 - (1 - e^{-\beta}) \psi_{s_i}^{k \to i}]
$$

#### Cavity free energy on trees

After addition of spin i and all the edges  $(ik)$  the free energy is changed by  $\Delta F^{i \to j}$ , which is given by the normalization

$$
Z^{i \to j} = e^{-\beta \Delta F^{i \to j}}
$$

In analogy the total free energy is

$$
F(\beta) = \sum_{i} \Delta F^{i} - \sum_{(ij)} \Delta F^{ij};
$$

where  $\Delta F^i$  is a free energy shift after addition of node i and all the edges around,  $\Delta F^{ij}$  is shift after addition of edge  $(ij)$ .

### From trees to sparse random graphs

The above equations are also correct on graphs with loops if the loops are long enough so that the clustering property holds (spins  $k$  are independent)

$$
\psi_{s_{k_1},s_{k_2}}^{k_1,k_2 \to i} - \psi_{s_{k_1}}^{k_1 \to i} \psi_{s_{k_2}}^{k_2 \to i} \to 0
$$

Does it hold?

- Math: proof for matching, coloring for  $\alpha < q$ , SAT for small  $\alpha$  etc.
- Physics: local self-consistency (stability) check, computation of the spin glass susceptibility

#### verage over graphs

Final order parameter is distribution  $\mathcal{P}(\psi_{s_i}^{i \to j})$  of  $\psi_{s_i}^{i \to j}$  over the graph, that is self-averaging (i.e. large graph is like average over graphs).

The self-consistent equation for  $\mathcal{P}(\psi_s^{i \to j})$  have to be solved numerically in general (population dynami
s).

#### Simplifications for coloring:

- Color symmetry not broken:  $\mathcal{P}(\psi_{s_i}^{i \to j})$  symmetric under color permutation.
- Factorization for regular graphs:  $\psi_{s_i}^{i \to j}$  the same for every edge, locally every edge have the same neighborhood.

## 1RSB: General idea

What if the clustering property does not hold?

- Simple case (ferromagnet): the pure phase decompose into few of them (magnetization positive, negative), within those the lustering property holds again!
- Less simple case (1RSB glass): the pure phase decompose into (exponentially) many, within those the clustering property holds again!

Is that correct?

- Math: No proof yet, the standard techniques for thermodynamical limit difficult, since with addition of one spin the system changes a lot. Less standard techniques are not far from success (Montanari, Semerjian, reconstruction on trees).
- Physics: local self-consistency (stability) check, computation of the spin glass sus
eptibility within states and in between states.

## 1RSB: What do we compute

Complexity function  $\Sigma(F)$  is entropy of states of internal free energy F. For computational reasons define "replicated" free energy as Legendre transform of the omplexity

$$
-\beta m\Phi(m,\beta)=-\beta mF(\beta)+\Sigma(F)
$$

What is  $m$ ?

- Legendre parameter, the same as temperature or chemical potential
- The Parisi replica symmetry breaking parameter
- Number of real replicas

What is the value of m?

• To minimize the total free energy of the system  $F + \Sigma(F)$  and keep the complexity  $\Sigma(F)$  positive  $\Rightarrow$  m = 1 or maximize the "replicated" free energy  $\Phi$ .

## 1RSB: Cavity equations

Order parameter on a single graph is survey (distribution)  $P(\psi_{s_i}^{i \to j})$  of probabilities  $\psi_{s_i}^{i \to j}$  for every edge (*ij*). Self-consistent equation

$$
P(\psi_{s_i}^{i \to j}) = \frac{1}{Z^{i \to j}} \prod_{k \in V(i) - j} \int dP(\psi_{s_i}^{k \to i}) \delta(\psi_{s_i}^{i \to j} - \mathcal{F}(\{\psi_{s_i}^{k \to i}\})) e^{-\beta m \Delta F^{i \to j}}
$$

Average over graphs: Distribution of distributions

Computational simplifications

- Zero temperature, only energetic terms integer fields! (Mulet, Pagnani, Weigt, Zecchina, 2002)
- At  $m=1$ , analogy with reconstruction on trees.
- Regular graph factorized case



## **End of the Technical Part**

## Results for coloring



- 1) Only one cluster, replica symmetry correct
- 2) Few entropically unimportant clusters appear, replica symmetry still orre
t
- 3) The large cluster truly splits into exponentially many small ones;  $m = 1$ , complexity  $\Sigma(m = 1) > 0$ , RS free energy still exact, dynamically glassy phase
- 4) The entropy condensed in a few clusters,  $m^*$  < 1, complexity  $\Sigma(m = 1)$  $m^*$ ) = 0, the true free energy larger than the RS one
- 5) No solutions anymore

## lgorithmic implications



- $1(+2)$  Monte Carlo like (simulated annealing, random walker search) algorithms work
	- 3) Monte Carlo like algorithms fails, Belief Propagation, the RS update of probabilities  $\psi_{s_i}^{i \to j}$  works!
	- 4) BP fails, Survey Propagation (Mézard, Zecchina, 2002), 1RSB update, works!
	- 5) No solutions anymore, different strategies for proving nonexistence of solution

### Few numbers and large q expansion



Erdös-Rényi graphs

	clust.	cond.	C()L
$q=4$	8.36	8.47	8.90
$a=5$	12.84	13.22	13.69

Leading terms in  $q \to \infty$ 

first cl.	clustering	condensation	COL/UNCOL
		$q \log q + q \log \log q + 2q \log q - \log q - 2 \log 2 + 2q \log q - \log q - 1$	



### Results for coloring





- Except the case of 3-coloring, the thermodynamically dominant clusters in the COL phase are stable (also at finite temperature)
- Intrinsically simpler than e.g. Sherrington-Kirkpatrick model, where FRSB holds, yet wide variety of unexpected transitions (given above, Back-bone like structures ...)

## Things we do not know yet

- Graphs with short loops!
- The region in 3-coloring which is not 1RSB stable
- The dynamics of decimation of the BP or SP
- More efficient solution of the non-simplified functional equations
- Clarify few things about the back-bone (hard fields), whitening procedure

# **Conclusions**

- In coloring (K-SAT etc.) variety of structural phase transitions
- Cavity method describes transitions exactly on random graphs, independently on any algorithm!
- Direct implication for design of efficient algorithms!
- The path towards a rigorous proof is quite advanced.

## Reference

Krzakala, Montanari, Ricci-Tersenghi, Semerjian, Zdeborova: Gibbs States and the Set of Solutions of Random Constraint Satisfaction Problems: to appear this week on cond-mat, submitted to PNAS.