Phase Transitions (and their meaning) in Random Constraint Satisfaction Problems

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Find these slides on my webpage:
www.pct.espci.fr/~florent/
Random Constraint Satisfaction Problems

- **Random K-Satisfiability**
  Consider $N$ boolean variables $x_i$ and $M$ random clauses of $K$ literals
  The average number of constraints is $\alpha = \frac{M}{N}$.
  Is it possible to find an assignment of the variables that satisfies all the constraints?
  Ex: Random 3-SAT

  $$(x_1 \lor \neg x_2 \lor x_3) \land (\neg x_2 \lor x_4 \lor x_5) \land (\neg x_6 \lor x_7 \lor \neg x_3) \land ...$$

- **Random q-Coloring**
  Consider $q$ colors, $N$ points and a random set of $M$ edges connecting them.
  Is it possible to color the points so that none of them has the same color as one of its neighbors?
  The average number of constraints is $\alpha = \frac{M}{N} = \frac{c}{2}$, where $c$ is the average connectivity.
  Ex: Random 3-COL

*COL and SAT are both NP-complete*
Example of CSP: the Coloring of a random graph

N=100 vertices, M=218 edges, average degree c=2M/N=4.36
Random Constraint Satisfaction Problems

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\[\text{COL and SAT are both NP-complete}\]
Why is random constraint satisfaction interesting?

Existence of a sharp SAT/UNSAT (or COL/UNCOL) threshold

- SAT/UNSAT threshold at average degree $\alpha_s$
- w.h.p. colorable for $\alpha < \alpha_s$ and w.h.p. uncolorable for $\alpha > \alpha_s$
- (A part of) Proof of existence (Friedgut 1997, Achlioptas, Friedgut, 1999)

Florent Krzakala

International Workshop on Statistical-Mechanical Informatics, Kyoto 2007
Why is random constraint satisfaction interesting?

Existence of a sharp SAT/UNSAT (or COL/UNCOL) threshold

- The time needed to decide satisfiability increases a lot close to $\alpha_s$

Computationally “hard” region near to the threshold

Data are from the same instances as Figure 3.
Why is \textit{random} constraint satisfaction interesting?

Existence of a sharp SAT/UNSAT (or COL/UNCOL) threshold

Can we compute the location of the COL/UNCOL threshold?

Are there other sharp transitions in the problem?

Why are some instances so hard? Is there a way to make them easy?
Consider the following Potts anti-ferromagnet Hamiltonian:

\[ H = \sum_{\langle ij \rangle} \delta(s_i, s_j) \]

A configuration with zero energy is a proper coloring.

To see if a graph is colorable just compute the ground-state energy and see if it is zero.

A random graph is locally tree-like with large loops (of typical size \( \log(N) \)): mean field methods are exact!

Coloring random graphs for physicist
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Random Constraint Satisfaction Problems such as \( q \)-COL of K-SAT can be studied within mean field spin glass theory using the “cavity method”

Overview

• Brief presentation of the cavity method

• Computation of the phase diagram

• Algorithmic consequences
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Statistical Physics of random CSP

Cavity approach: A mean field method for statistical physics models on tree-like graphs.
Equivalent to the replica method of disordered systems

Parisi, Mézard, Virasoro ‘87, Parisi, Mézard ’00,

Accomplishments
Statistical Physics of random CSP

Cavity approach: A mean field method for statistical physics models on tree-like graphs. Equivalent to the replica method of disordered systems

Accomplishments

Prediction of a glassy (clustered) phase in the colorable region

Mézard, Zecchina, Parisi, ‘02, Biroli, Monasson, Weigt, ‘99

The exact SAT/UNSAT threshold computed. Survey Propagation algorithm designed.

K-SAT: Mézard, Zecchina, Parisi, ‘02,
q-COL: Mulet, Pagnani, Weigt, Zecchina, ‘03
What are clusters?

- **Roughly said**: Lumps (groups) of nearby solutions which are in some sense disconnected from each other.
- **For mathematical physicist**: “Extremal Gibbs measures = pure states”.
- **For computer scientist**: Fixed points of belief propagation.
- **For spin glass physicist**: Solutions of TAP equations.
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What is the distribution of the sizes of the clusters?
A refined analysis of clusters

- **Entropy (size) of a cluster** $s$:
  logarithm of the number of solutions belonging to the cluster (divided by the number of variables).

- **Complexity function** $\sum(s)$:
  logarithm of the number of clusters of size $s$

$$\sum(s) = e^{N\sum(s)}$$

If $\sum(s) > 0$, there are exponentially many states of size $s$.
If $\sum(s) < 0$, then states of size $s$ become exponentially rare as $N$ grows.
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  If $\Sigma(s) > 0$, there are exponentially many states of size $s$.
  
  If $\Sigma(s) < 0$, then states of size $s$ become exponentially rare as $N$ grows.

- We compute the complexity function using the zero temperature cavity method via a Legendre transform $\Phi(m)$ of $\Sigma(s)$.

  **Main idea** (Mézard, Palassini, Rivoire, ’05): weight each cluster by its size to the power $m$:

  $$
  e^{N\Phi(m)} = \sum_\alpha (e^{Ns_\alpha})^m = \int e^{N[ms + \Sigma(s)]} \, ds \\
  \Phi(m) = ms + \Sigma(s), \quad \frac{\partial \Sigma(s)}{\partial s} = -m
  $$

  **Note:** the approach of Mézard, Zecchina, Parisi ‘02; Mulet, Pagnani, Weigt, Zecchina ‘02 was at $m=0$. 

Solve (mostly numerically) the 1RSB cavity equations

+ Work out the several special cases when the equations simplify
  \((m=1, m=0, \text{frozen variables, regular graphs} \ldots)\)
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Learning from $\Sigma(s)$

Example of 6-coloring, connectivities 17, 18, 19, 20 (from top).
6 coloring of regular random graph

very low connectivity
6 coloring of regular random graph

connectivity \( c=17 \)
6 coloring of regular random graph    connectivity $c=18$
6 coloring of regular random graph

connectivity $c=19$
6 coloring of regular random graph

connectivity $c=20$
Many phase transitions
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Clustering transition

The phase space splits into exponentially many states

\[ c_d(3) = 4, \quad c_d(4) = 8.35, \quad c_d(5) = 12.84 \]
Many phase transitions

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★ Condensation transition
- Entropy dominated by finite number of the largest states.
  \[ c_c(3) = 4, \quad c_c(4) = 8.46, \quad c_c(5) = 13.23 \]
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**COL/UNCOL transition**
- No more clusters, uncolorable phase
  \[ c_s(3) = 4.69, \quad c_s(4) = 8.90, \quad c_s(5) = 13.67 \]
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Moreover: The entropically dominating clusters are **1RSB stable in the colorable phase**
(at least for \( q > 3 \))
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(at least for q>3)
The freezing of clusters

Two types of clusters are found

**Soft or “unfrozen” clusters**

All variables are allowed at least two different colors in the cluster

**Hard or “frozen” clusters**

A finite fraction of variables are allowed **only one color** in all solutions belonging to the cluster: we say that these variables “freeze”
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☆ Rigidity transition

Frozen variables appears in the dominating states.

\[ c_r(3) = 4.66, \ c_r(4) = 8.83, \ c_r(5) = 13.55 \]
The phase transitions

🌟 Clustering/Dynamic transition

🌟 Condensation/Static transition

🌟 COL/UNCOL transition

🌟 Freezing of clusters and the rigidity transition
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- Clustering/Dynamic transition
- Condensation/Static transition
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- **Clustering/Dynamic transition**
  - “Ergodicity breaking transition”, equilibration time diverges
  - Metropolis Monte-Carlo inefficient for sampling

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Easy/Hard transition for the “MC sampling” problem (but not for the “solving” problem)
Meaning of the transitions

★ Clustering/Dynamic transition
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- Metropolis Monte-Carlo inefficient for sampling
★ Condensation/Static transition
- “Static replica symmetry breaking transition”
- Many clusters exist, but a finite number of them covers almost all solutions
- The overlap function $P(q)$ becomes non-trivial
★ COL/UNCOL transition
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  - No solutions exist anymore

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![Diagram showing transitions]

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  - Solutions are hardly constraint within the cluster
  - For $c>c_r$, most solutions belong to frozen clusters

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The frozen clusters are responsible for the difficulty of finding solutions (not the clustering in itself).

Easy/Hard transition for the “MC sampling” problem (but not for the “solving” problem)
“Wet toes” algorithm

Arkless strategy for flood victims

You are on a rugged landscape that is being flooded
“Wet toes” algorithm

Arkless strategy for flood victims

Water goes up. When your toes are wet step back on the land!
“Wet toes” algorithm

Arkless strategy for flood victims

And wait until your toes get wet again...
“Wet toes” algorithm

Arkless strategy for flood victims

Sooner or later you’ll find yourself on a smaller island...
“Wet toes” algorithm

Arkless strategy for flood victims

Then even a smaller one...
“Wet toes” algorithm

Arkless strategy for flood victims

Until eventually you’ll drown (if you can’t swim!)
“Wet toes” algorithm

Arkless strategy for flood victims

Finally, all land will be flooded!
“Wet toes” algorithm

Add links one by one and use a local algorithm to solve contradictions

The algorithm works until the cluster disappears.
**Frozen clusters make it hard!**

Add links one by one and use a local algorithm to solve contradictions.

- **A fundamental properties of frozen clusters:**
  - Frozen clusters are fragile and disappear after the addition of few links.
  - The number of needed changes is finite in unfrozen clusters and infinite in frozen ones. *Semerjian ‘07*
Frozen clusters make it hard!

Add links one by one and use a local algorithm to solve contradictions.

The algorithm works until the cluster disappears and this happens when frozen variables appear.
Performance of the “Wet toes” algorithm

Goes beyond the dynamical and the condensation transition for $q=3$ & 4
Performance of the “Wet toes” algorithm

Goes beyond the dynamical and the condensation transition for q=3 & 4

But stops before the rigidity transition!
Another example: Walk-COL algorithm

(1) Randomly choose a spin that has the same color as at least one of its neighbors.
(2) Change randomly its color. Accept this change with probability one if the number of unsatisfied spins has been lowered, otherwise accept it with probability $p$.
(3) If there are unsatisfied vertices, go to step (i) unless the maximum running time is reached.
Conclusions & perspectives

Determination of the phase diagram of the random coloring problem. A rich “glassy”-like phenomenology is found:
- dynamical transition
- condensation/Kauzmann transition
- “rigidity/freezing” transition
- COL/UNCOL transition

Discussion of the algorithmic implications
Frozen variables are responsible for the computational hardness

Future directions:
- More (and possibly exact) results on the EASY/HARD transition and frozen clusters? See next talk by F. Zamponi
- Toward a rigorous formulation of the cavity results? Numerical check of static and dynamic predictions?
  - Enumeration (c.f. Last talk by A. Hartmann)
  - Monte-Carlo simulations?
- Better algorithms using message passing (BP and SP)?
Monte-Carlo simulations?

The typical phase diagram in a temperature/connectivity plane

Is it possible to confirm these predictions in a Monte-Carlo simulation and to find the dynamic, static and Gardner transition?
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Message Passing algorithms beyond SP?

- Survey Propagation (cavity recursion on a single graph at m=0) is currently the best solver for random SAT
- Belief Propagation (replica symmetric cavity recursion on a single graph) can also be used with very good results (as it actually asymptotically gives exact marginals until the condensation)

What is the limit of these algorithms?
What is the best way to use message passing in order to find a solution?

See the recent paper by Montanari et al. arxiv:0709.1667
References


L. Zdeborová and FK: Phase Transitions in the Coloring of Random Graphs, Accepted in *PRE*, arXiv:0704.1269

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Thanks to the organizers for their kind invitation...

どうもありがとうございました。
References


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... and to the audience for your attention.
Bonus Section
Large number of colors (analytical results)

\[
\begin{align*}
\text{SP nontrivial} & \quad c_{SP} \simeq q (\log q + \log \log q + 1 - \log 2) \\
\text{Clustering} & \quad c_r \simeq q (\log q + \log \log q + 1) \\
\text{Rigidity} & \quad c_g \simeq 2q \log q - \log q - 2 \log 2 \\
\text{Condensation} & \quad c_q \simeq 2q \log q - \log q - 1 \\
\end{align*}
\]
The Cavity Method

Parisi, Mézard, Virasoro ‘87
Parisi, Mézard ‘00
Parisi, Mézard, Zechinna ‘02
The iterative solution on a tree

Coloring = anti-ferromagnetic Potts model at zero temperature

Recursive equations on a tree (Belief propagation):

\[ \psi_{s_i}^{i \to j} = \frac{1}{Z^{i \to j}} \prod_{k \in V(i) \setminus j} \sum_{s_k} (1 - \delta_{s_is_k}) \psi_{s_k}^{k \to i} \]

\[ = \frac{1}{Z^{i \to j}} \prod_{k \in V(i) \setminus j} (1 - \psi_{s_i}^{k \to i}) \]

\( \psi_{s_i}^{i \to j} \) is the set of probabilities that the spin i takes the color q in absence of the spin j
The replica symmetric solution on a graph

A random graph being locally tree-like, assume a “fast” decay of correlations, then the RS solution should be correct.
The replica symmetric solution on a graph

A random graph being locally tree-like, assume a “fast” decay of correlations, then the RS solution should be correct.

Rigorously proven for regular random graphs for $c < q-1$...

Bandyopadhyay, Gamarnik ‘05

... and believed to be correct even beyond (until $c \sim q \log q$).
The replica symmetric solution on a graph

A random graph being locally tree-like, assume a “fast” decay of correlations, then the RS solution should be correct.

Rigorously proven for regular random graphs for \( c < q-1 \)....

... and believed to be correct even beyond (until \( c \sim q \log q \)).

Solution of the self-consistent equation:
Only the “paramagnetic” \( \psi = (1/q, 1/q, \ldots) \) in the COL phase.

This leads to the following entropy:

\[
\begin{align*}
    s_{RS} &= \log q + \frac{c}{2} \log \left( 1 - \frac{1}{q} \right)
\end{align*}
\]
When is the tree solution expected to be correct?

If we are in a “paramagnetic phase”.

From spin glass theory, we expect however a transition to a spin glass phase.

1) Continuous transition (divergence of the Spin glass susceptibility) like in the Sherrington-Kirkpatrick model

2) Discontinuous transition (like in the p-spin or the Random Energy model model)
Replica symmetry breaking

The phase space splits into an exponential number $\mathcal{N}$ of components. Define the complexity (or configurational entropy) $\sum_{\alpha} \mathcal{N}$ as $\mathcal{N} = e^{N\Sigma}$.

The complexity can be computed using a "modified" partition sum:

$$\sum_{\alpha} Z_{\alpha}^m = \sum_{\alpha} \left( \sum_{s \in \alpha} e^{-\beta E(s)} \right)^m = \int dfe^{-N(\beta mf(\beta) - \Sigma(f))} = e^{-\beta mN \Phi(\beta,m)}$$
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The “Replicated” free energy is the Legendre transform of the complexity

$$-\beta m \Phi(m, \beta) = -\beta m F(\beta) + \Sigma(F)$$
The replica symmetry breaking recursion

Order Parameter:
Probability distribution $P^{i \rightarrow j}(\psi)$ of fields for every edge.

Self-consistent equation:

$$P^{i \rightarrow j}(\psi) = \frac{1}{Z^{i \rightarrow j}} \int \delta[\psi_{s_i}^{i \rightarrow j} - \mathcal{F}(\{\psi_{s_i}^{k \rightarrow i}\})] e^{m \Delta S^{i \rightarrow j}} \prod_{k \in V(i) - j} dP^{k \rightarrow i}(\psi)$$
The replica symmetry breaking recursion

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\]

Numerical Solution - Population dynamics: very heavy!!!

Simplifications : m=0, m=1, regular graphs, hard fields...

Large q expansion