Phase Transitions in Optimization Problems

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Göttingen, november 2004

Combinatorial optimization

- Configurations : N discrete variables (e.g. Boolean $s_i \in \{0, 1\}$)

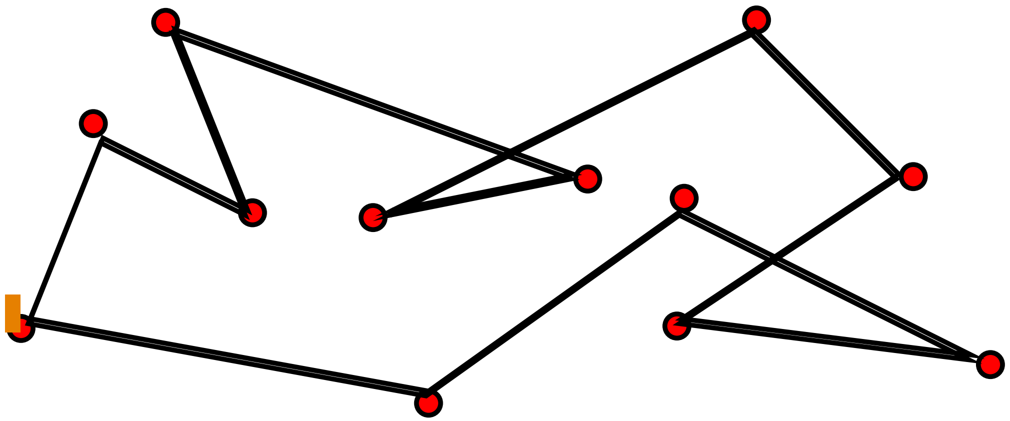
- Energy (cost) function $E(\mathcal{C})$; typically computable in $\sim N^b$ operations.

- Optimization Pb: Find $\mathcal{C}^*$ which minimizes $E(\mathcal{C})$.
  Evaluation Pb: Find the cost $E(\mathcal{C}^*)$.
  Decision Pb: Is there a $\mathcal{C}$ with $E(\mathcal{C}) < E_0$?

Examples: Travelling Salesman Problem, Assignment, Spin glass, Eulerian circuit, Hamiltonian cycle, Colouring, Satisfiability,...

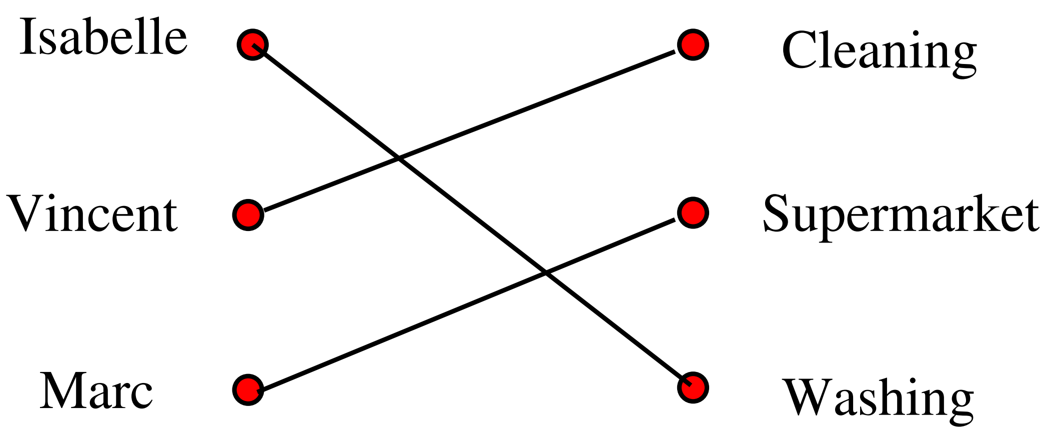
Examples

1) Travelling Salesman Problem



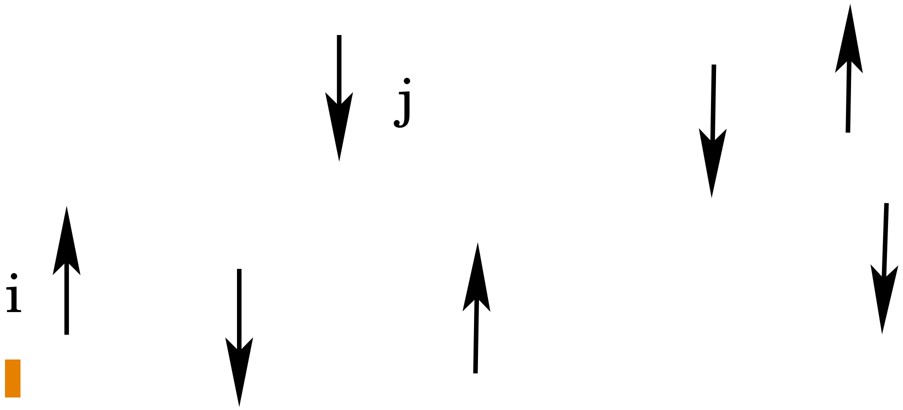
N points
$\mathcal{C}$ = tour; $(N-1)!/2$
$E(\mathcal{C})$ = length

2) Assignment



N persons, N jobs
$\mathcal{C}$ = assignment; $N!$
$E(\mathcal{C}) = -\sum$ affinities

3) Spin glass



N spins

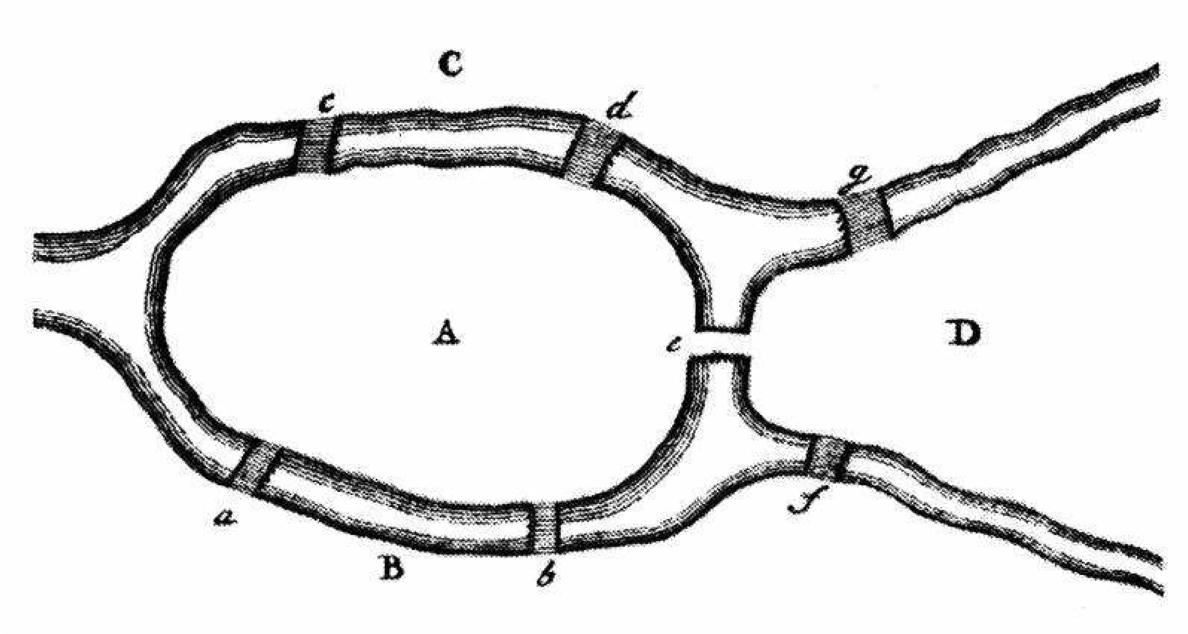
$\mathcal{C}$ = spin configuration; 2^N

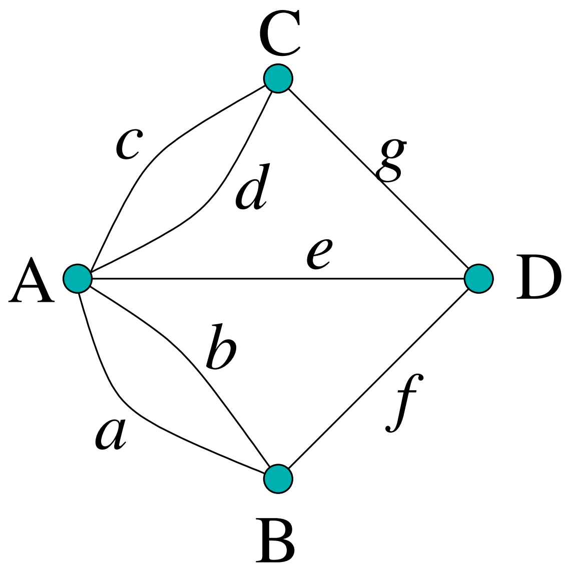
$E(\mathcal{C}) = -\sum J_{ij}\sigma_i\sigma_j$

4) Eulerian circuit

5) Hamiltonian path

Eulerian circuit



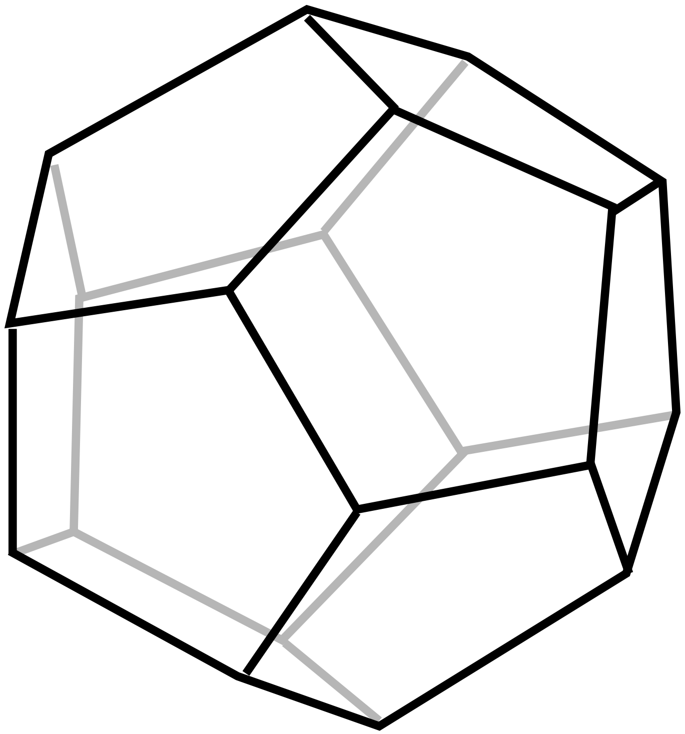


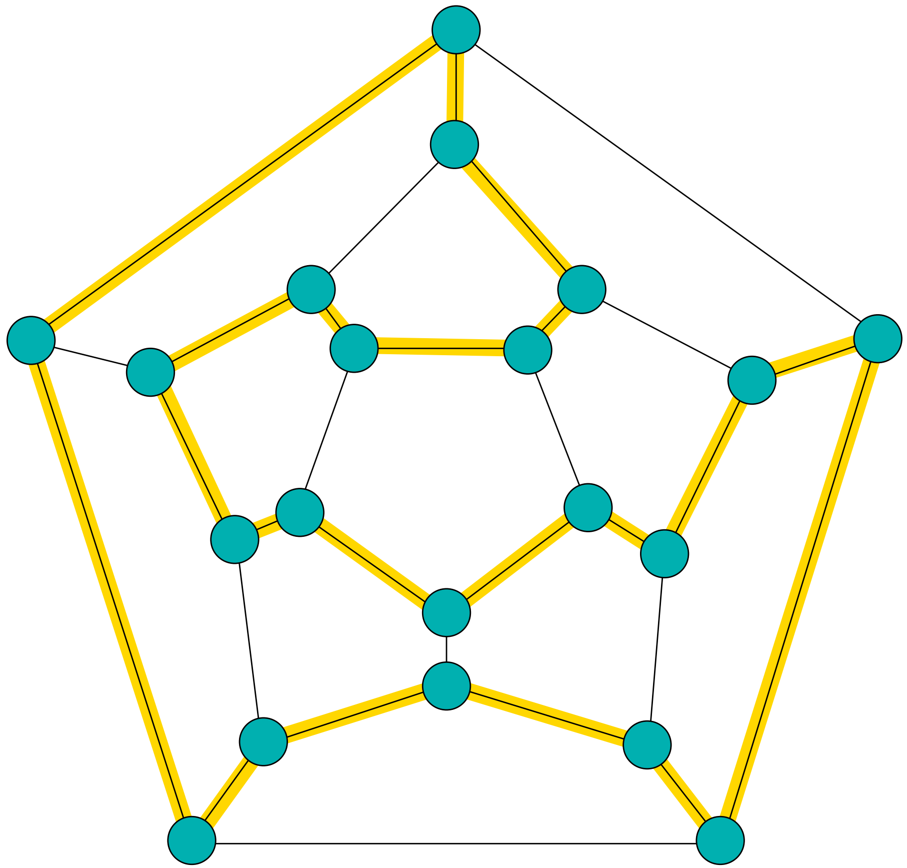
Königsberg seven bridges

Euler 1736:

- Graph, visit all edges once and only once.
- Eulerian circuit $\Longleftrightarrow$ every vertex has even degree

Hamiltonian path





Hamilton's Icosian game (Sir William, Astronomer Royal of Ireland, 1859): Find a route along the edges, visiting each corner exactly once and returning to the starting corner. No simple solution...

Classification: computational complexity

Worst case analysis of decision problems

P $=$ polynomial $\leftrightarrow$ tractable, $t < N^{\alpha}$. Ex: Assignment, Eulerian circuit, Spin glass in $d = 2$, Random Field Ising Model,...

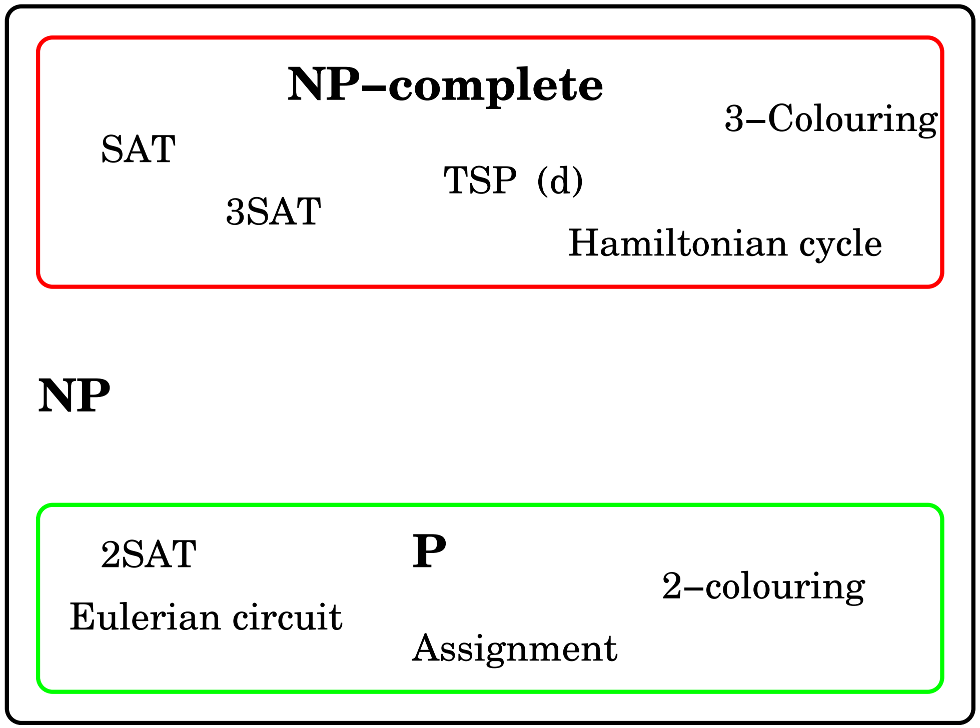
NP $=$ non-deterministic polynomial (A 'yes' solution can be checked in polynomial time) $\leftrightarrow$ many problems!

NP-complete: the hardest **NP** problems. Problem A is **NPC** iff all problems in **NP** are polynomially reducible to it. (If A is solvable in polynomial time, all problems in **NP** are solvable in polynomial time).

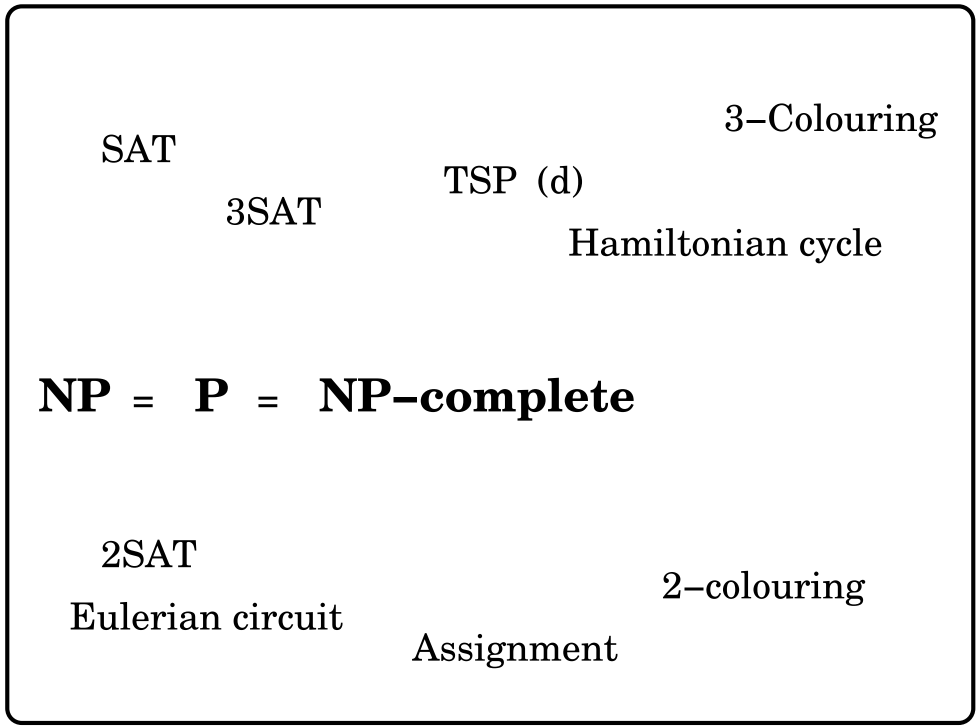
Theorem (Cook, 1971): The SATISFIABILITY problem is NP-complete.

Other NPC: 3SAT, TSP, Hamiltonian cycle, Spin glass in $d \geq 3$,..

P = NP ?



Conjectured



Possible

SATISFIABILITY: an example

"You are chief of protocol for the embassy ball. The crown prince instructs you either to invite Peru or to exclude Qatar. The queen asks you to invite either Qatar or Romania or both. The king, in a spiteful mood, wants to snub either Romania or Peru or both. Is there a guest list that will satisfy the whims of the entire royal family?" (from B.Hayes, American Scientist 1997).

Configurations = assignments of Boolean variables: $P, Q, R \in \{0, 1\}$

Constraints = clauses: $P \vee \bar{Q},\ Q \vee R,\ \bar{R} \vee \bar{P}$

Is there a choice of P, Q, R such that all constraints are satisfied (SAT)?

SATISFIABILITY: an important problem

2^N Configurations= assignments of N Boolean variables: $x_i \in \{0, 1\}$

M Constraints $=$ clauses like $x_1 \vee x_{27} \vee \bar{x}_3, \quad \bar{x}_{11} \vee x_2, \ ....$

Decision problem: is there a choice of the Boolean variables such that all constraints are satisfied (SAT)?

Generic (conjunctive normal form $(x_1 \vee x_{27} \vee \bar{x}_3) \wedge (\bar{x}_{11} \vee x_2) \wedge \ldots$).

NP-complete

Constraint satisfaction problems: Many discrete variables, many constraints, is there a choice of variables which satisfies all constraints? Ubiquitous.

"Worst-case" versus "Typical-case" complexity

Computational complexity = worst case analysis.

Experimental complexity = typical case analysis: $\longrightarrow$ class of samples (probability measure on instances). Example: CuMn at one percent Mn

Ex : Complexity of the random 3SAT problem. Three variables per clause, chosen randomly in $\{x_1, .., x_N\}$, negated randomly with probability $1/2$:

$$(x_1 \vee x_{27} \vee \bar{x}_3) \wedge (\bar{x}_{11} \vee x_3 \vee x_2) \wedge \ldots \wedge (x_9 \vee \bar{x}_8 \vee \bar{x}_{30})$$

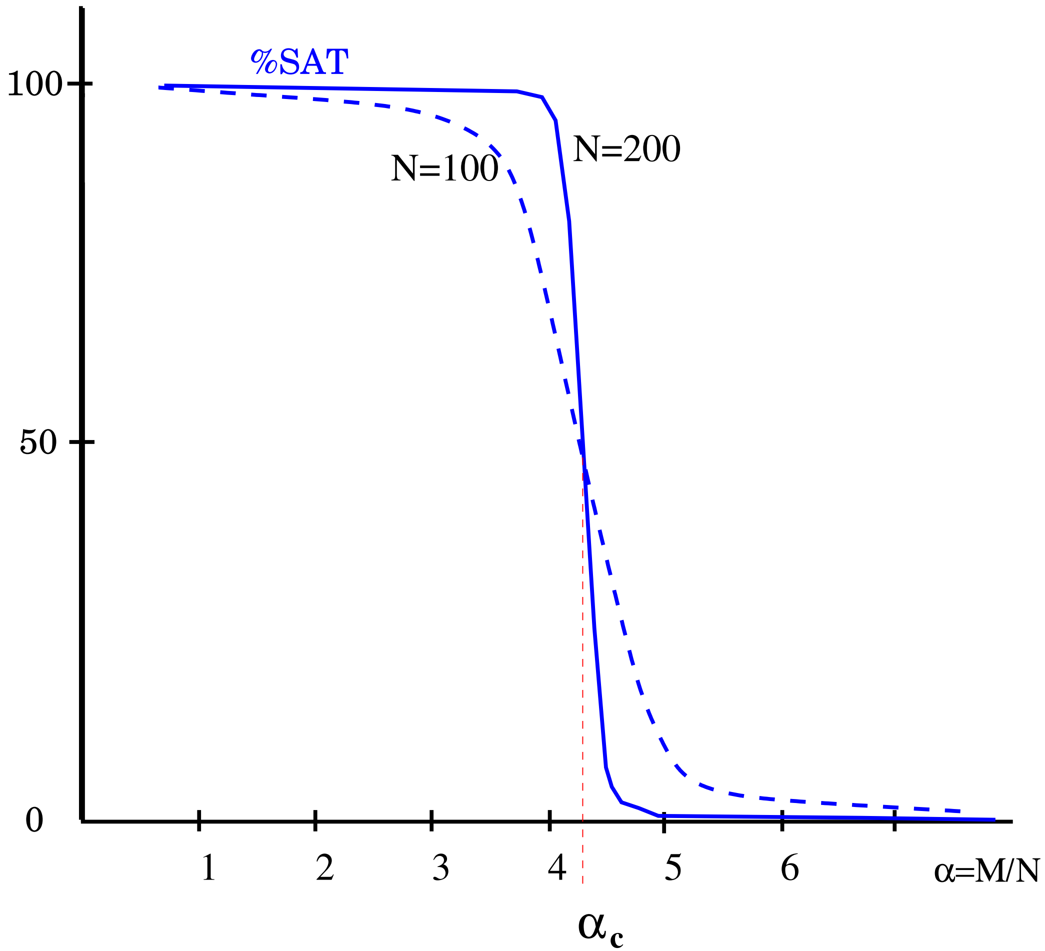
Control parameter: $\alpha = \frac{M}{N}$= Constraints/Variables.

Numerically:Threshold phenomenon at $\alpha_c \sim 4.26$.

Numerics Mitchell Selman Levesque Kirkpatrick Crawford Auton...;

Threshold Friedgut; **Bounds** Kaporis Kirousis Lalas Dubois Boufkhad...

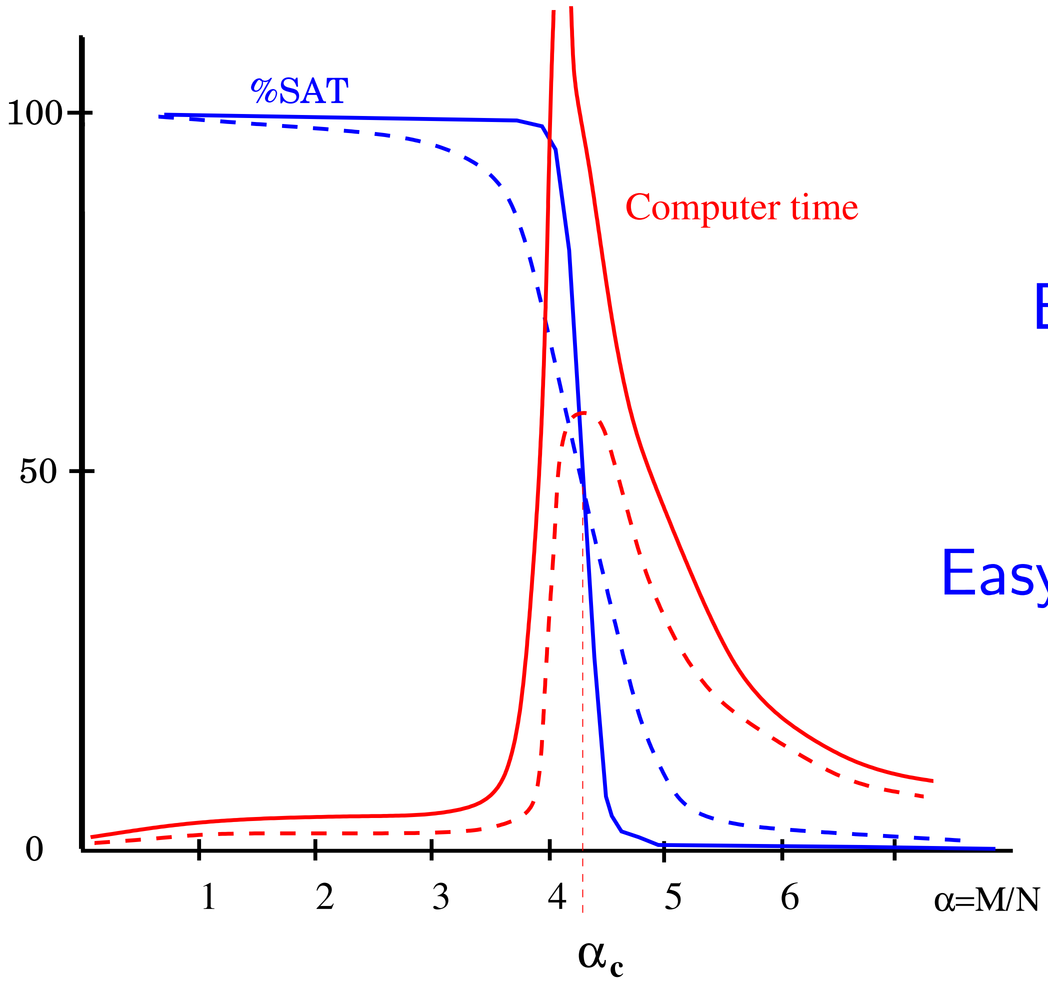
Threshold phenomenon → Phase transition



generically SAT for $\alpha < \alpha_c$

generically UNSAT for $\alpha > \alpha_c$

Threshold phenomenon → Phase transition



Easy, and generically SAT, for $\alpha < \alpha_c$

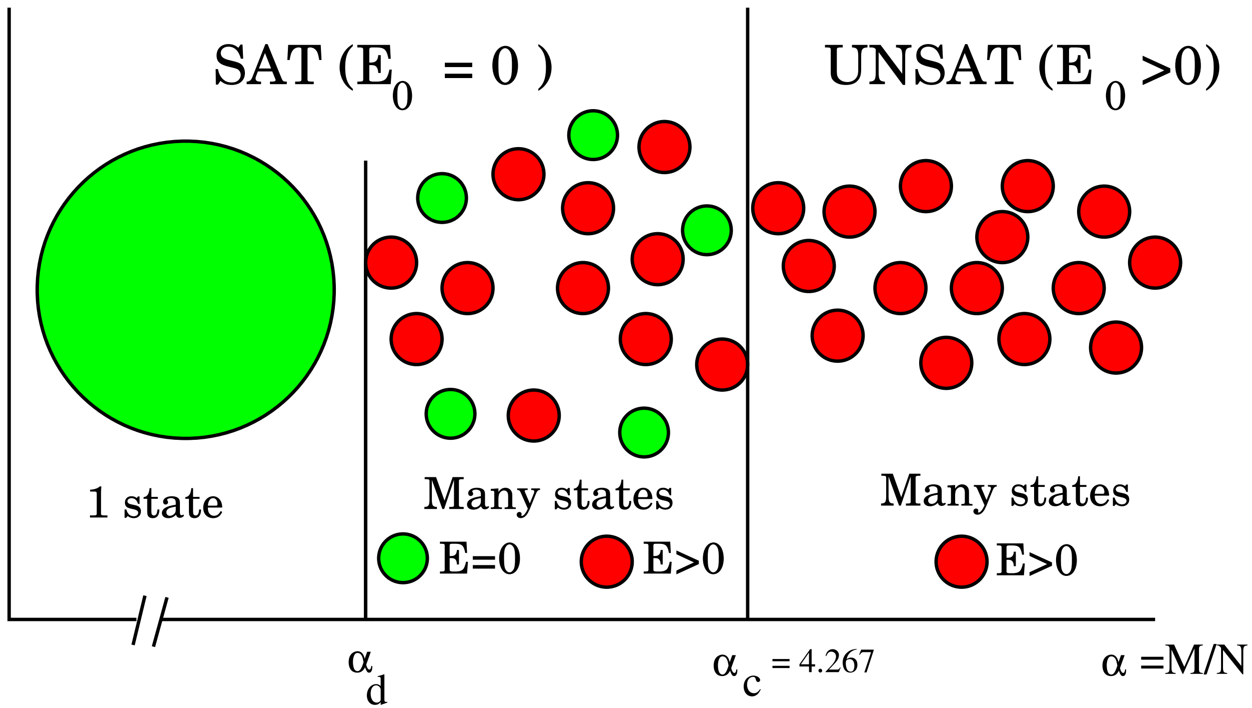
Hard, in the region $\alpha \sim \alpha_c$

Easy, and generically UNSAT, for $\alpha > \alpha_c$

Statistical physics of the random 3-SAT problem

Monasson, Zecchina, Weigt, Biroli, ..., MM, Parisi, Zecchina: $\longrightarrow$ Phase diagram + New algorithm.

1- Analytic result: Three phases   2- New algorithm: Survey propagation



Increasing α:

Easy-SAT, Hard-SAT,

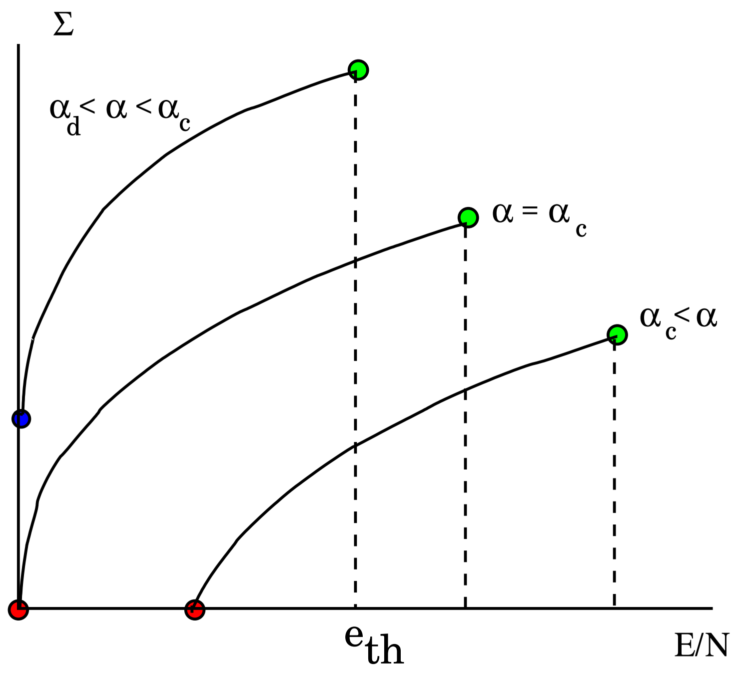
UNSAT

States and complexity

Minimum Energy Configurations: energy cannot be lowered by a finite number of flips

State/Cluster= { MEC connected by finite flips }.

Proliferation of states: At $\alpha > \alpha_d$, many states: $\mathcal{N}(E) \sim \exp\left(N\Sigma\left(\frac{E}{N}\right)\right)$



$\Sigma(0) \longrightarrow$ clusters of SAT configurations

$\Sigma(e_{th}) \longrightarrow$ metastable clusters

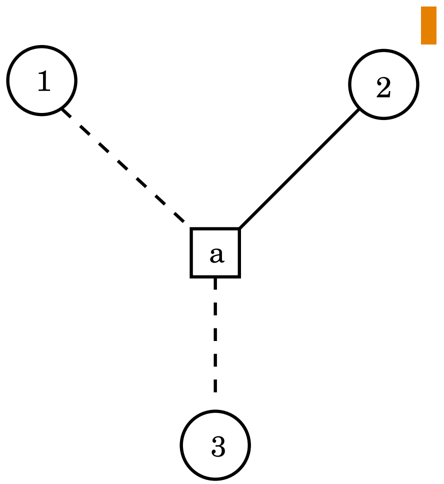
Main steps

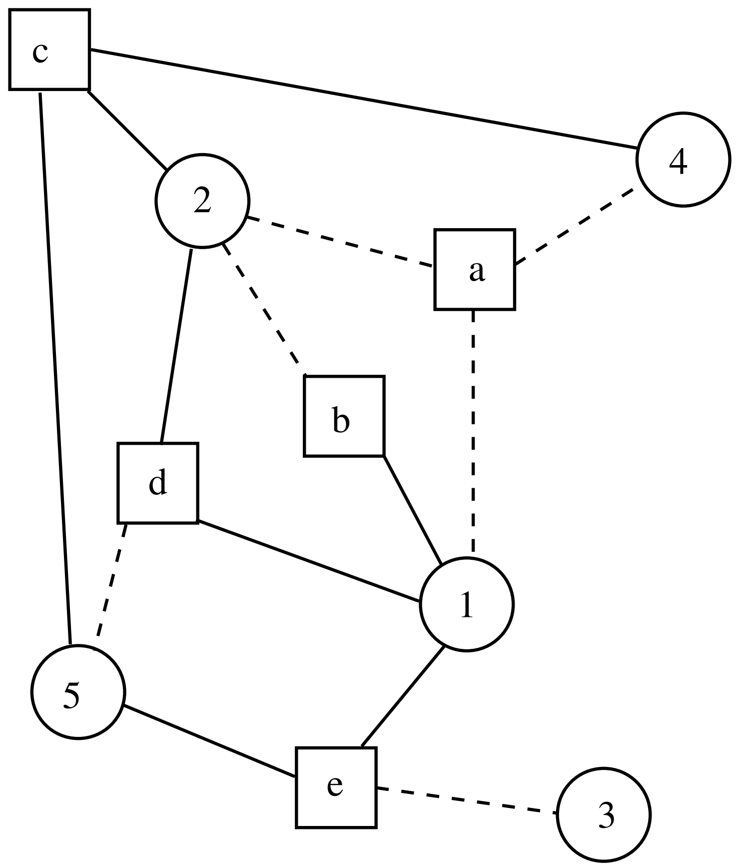
- Graphical representation: 3SAT as a random factor graph
- Elementary message passing procedure: (Bethe approximation at zero temperature): exchange of warnings between constraints and variables.
- In the presence of many clusters: cavity method $\longrightarrow$ messages $=$ surveys of elementary messages in all clusters.

Graphical representation: "factor graph"

One clause a:

Boolean: $\bar{x}_1 \vee x_2 \vee \bar{x}_3$



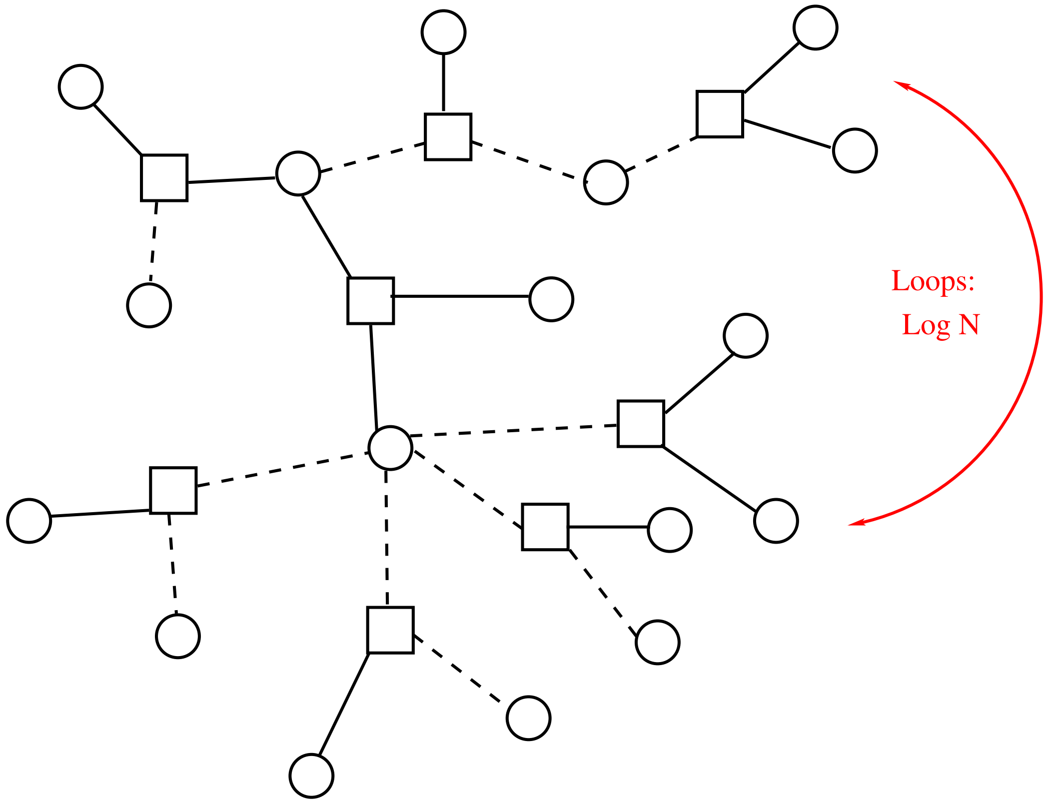


$$(\bar{x}_1 \vee \bar{x}_2 \vee \bar{x}_4) \wedge (x_1 \vee \bar{x}_2) \wedge (x_2 \vee x_4 \vee x_5)$$

$$\wedge (x_1 \vee x_2 \vee \bar{x}_5) \wedge (x_1 \vee \bar{x}_3 \vee x_5)$$

Geometry of the random 3-SAT graph: tree-like structure

→ Random bipartite graph:



Locally tree-like.

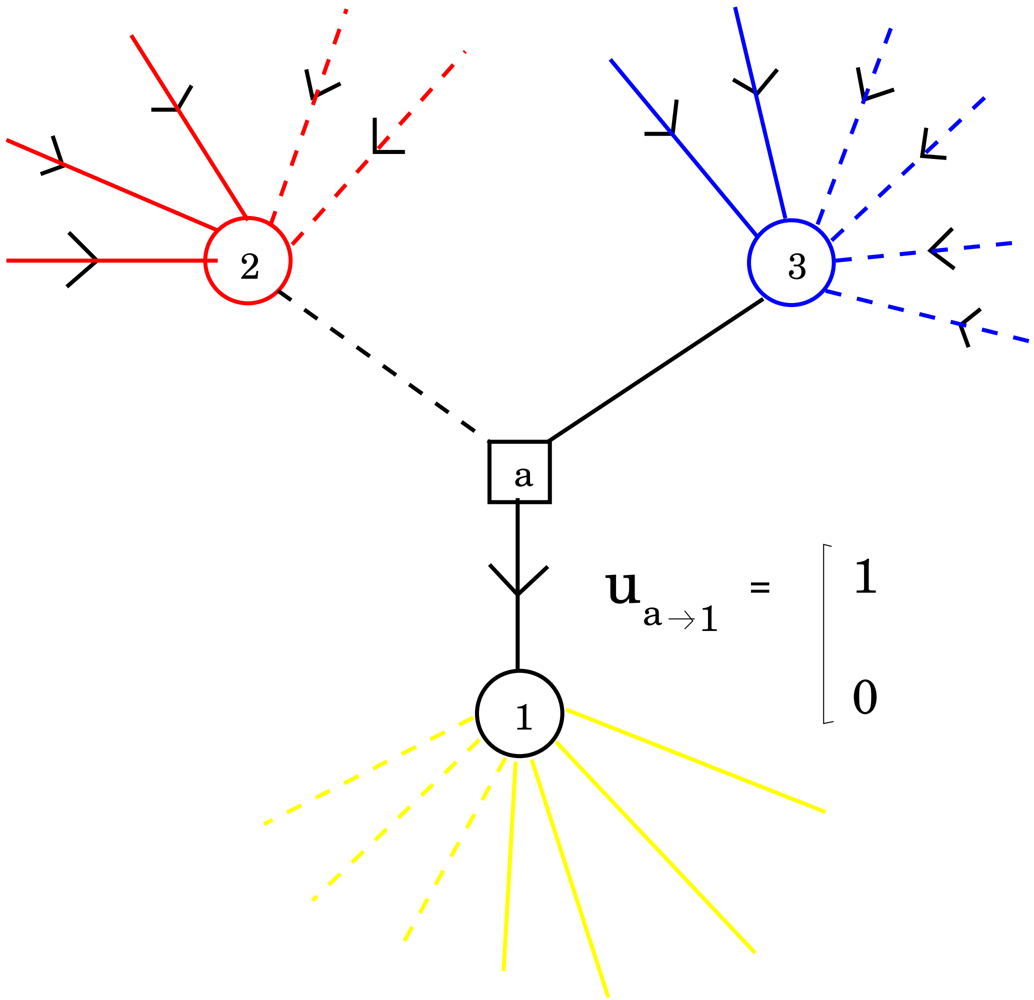
→ Iterative methods

Frequent situation:

finite connectivity random graphs

(e.g. Tanner graphs for LDPC codes)

Simple message passing: warning propagation

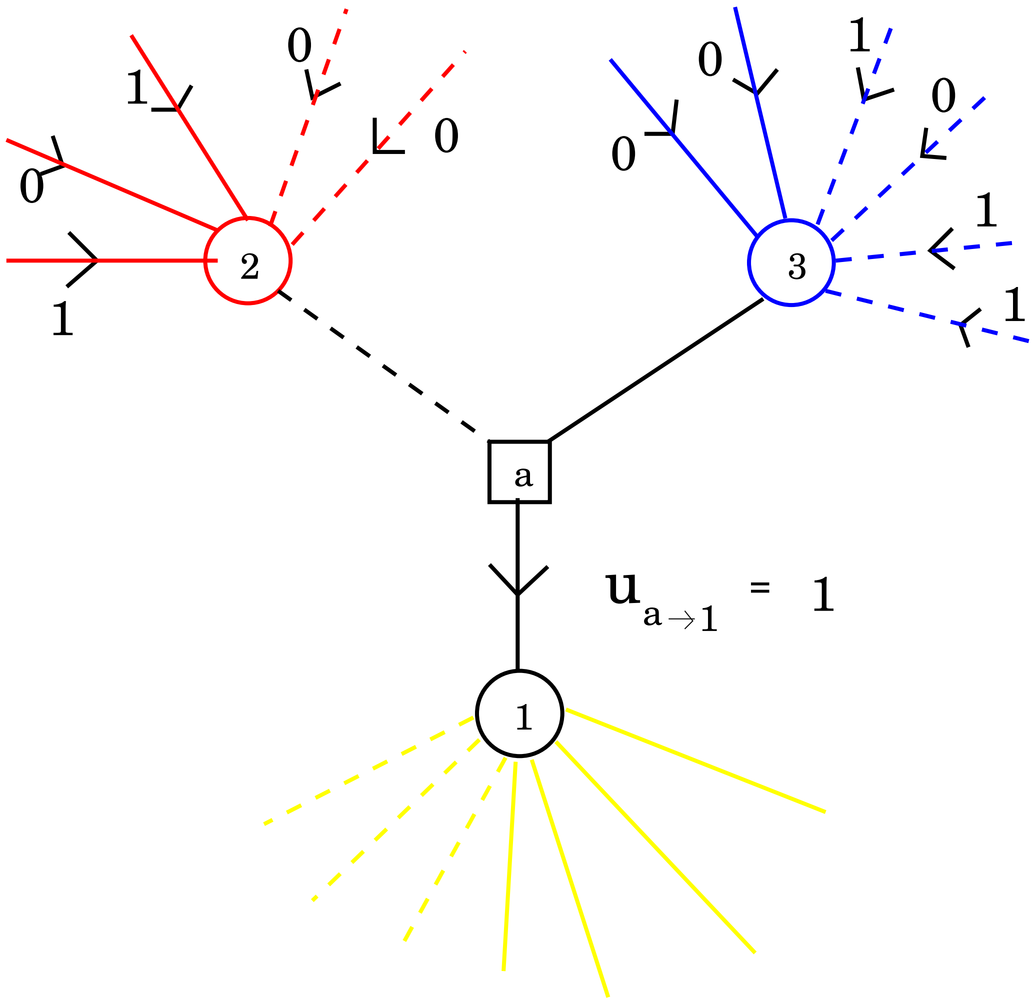


Message $u_{a\to 1} \in \{0, 1\}$

sent from clause a

to variable 1

Simple message passing: warning propagation



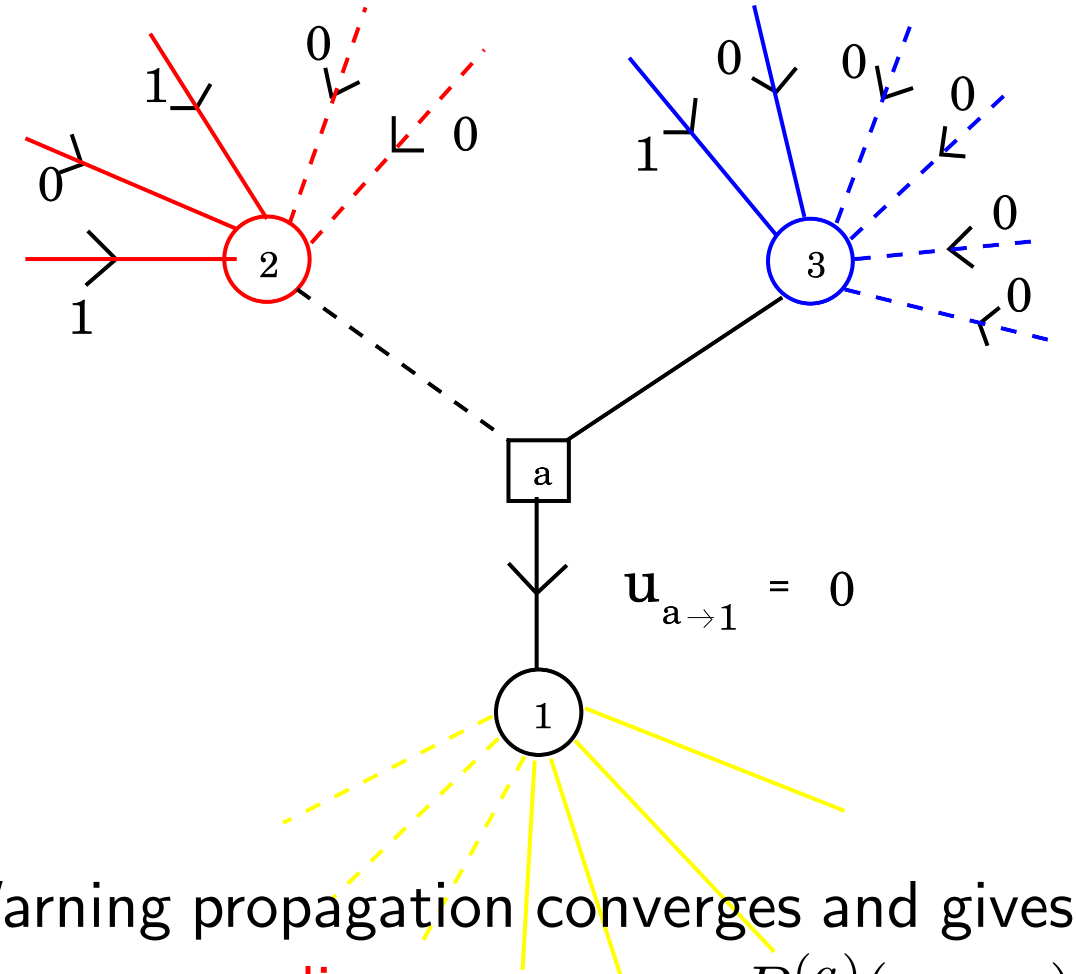
Warning $u_{a\to i} = 1$:

"According to the messages

I received, you should take the

value which satisfies me!".

Simple message passing: warning propagation

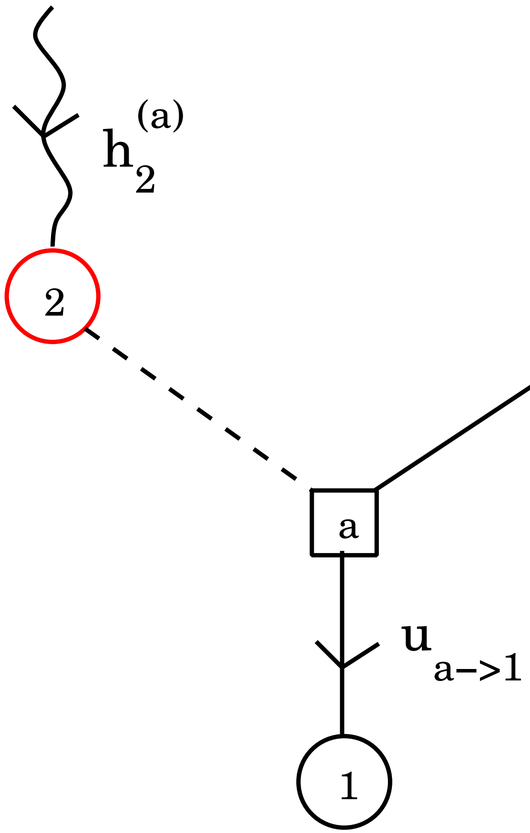


No warning $u_{a \to i} = 0$:

"No problem, take any value!"

Warning propagation converges and gives the correct answer on a tree: SAT iff no contradictory message $P^{(a)}(x_2, x_3) \sim P^{(a)}(x_2) P^{(a)}(x_3)$

Statistical physics analogue: Bethe approximation at $T = 0$



$$P(s_1, s_2, s_3) \propto e^{-\beta\left[E_a(s_1,s_2,s_3) - h_1^{(a)} s_1 - h_2^{(a)} s_2 - h_3^{(a)} s_3\right]}$$

$$P_{cavity}(s_1) \propto \sum_{s_2,s_3} e^{-\beta\left[E_a(s_1,s_2,s_3) - h_2^{(a)} s_2 - h_3^{(a)} s_3\right]}$$

$$\rightarrow P_{cavity}(s_1) \propto e^{-\beta\left[u_{a\rightarrow 1}\left(h_2^{(a)}, h_3^{(a)}\right) s_1\right]}$$

$$h_2^{(a)} = \sum_{b \neq a} u_{b \rightarrow 2}$$

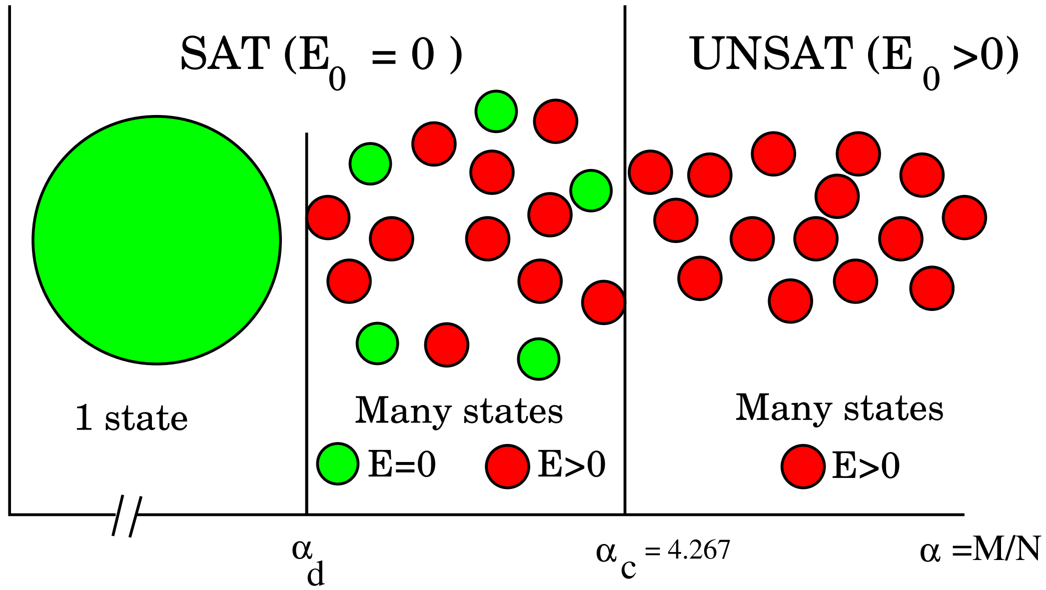
Proliferation of states

Warning propagation works if one can neglect the correlations between the input fields (tree).

Random 3SAT "locally tree-like": generically, x_2 and x_3 are very far away (distance $O(\log(N))$) $\longrightarrow$ Uncorrelated if only one cluster / pure state.

$\longrightarrow$ OK in Easy-SAT phase.

$\longrightarrow$ Wrong in Hard-SAT phase



From warning propagation to survey propagation

From the Bethe approximation to the Cavity method

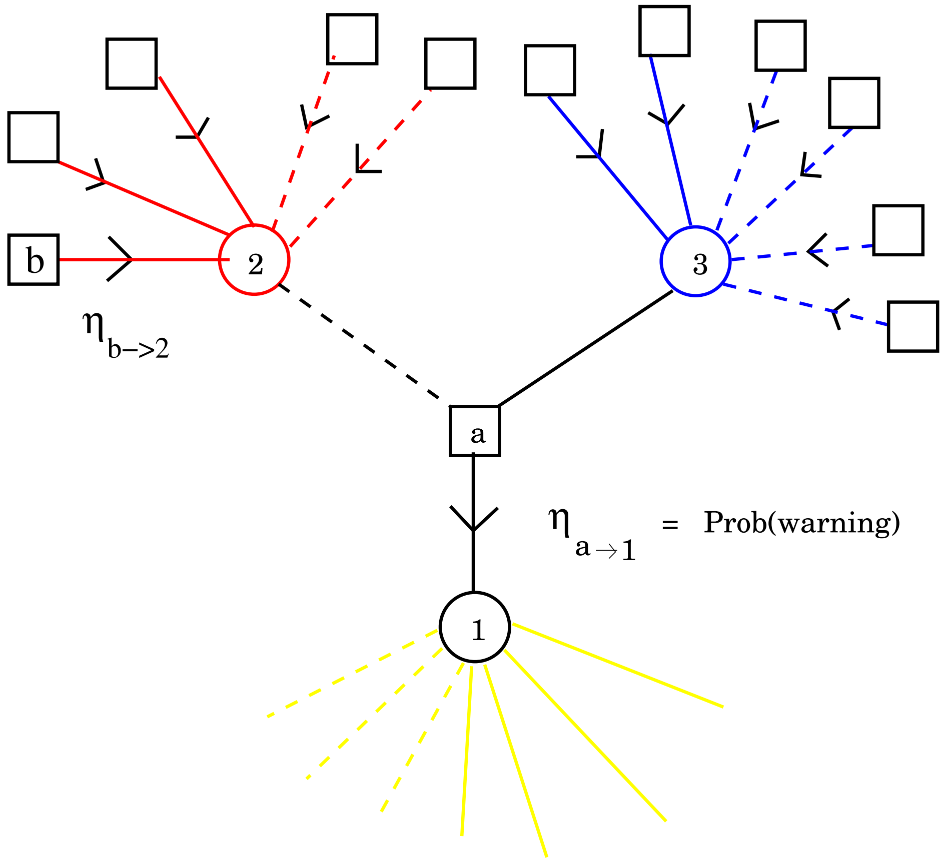
Hard SAT phase: Message $=$ Survey of the elementary messages in the various clusters of SAT configurations: $\eta_{a \to i} =$ probability of a warning being sent from constraint a to variable i, when a cluster is picked up at random.

$\longrightarrow$ Propagate the surveys along the graph. Converges!

$\longrightarrow$ Results on the phase diagram and the complexity, from the statistical analysis of the distribution of surveys in a generic sample.

$\longrightarrow$ Information on a single sample: a local field on each variable $\longrightarrow$ new algorithmic strategies

Survey propagation

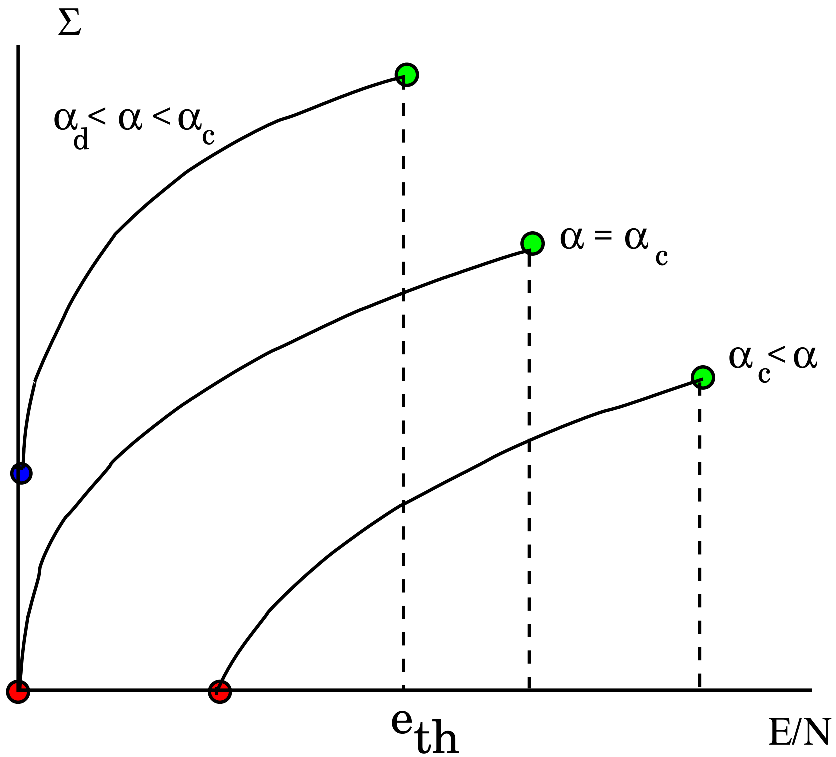


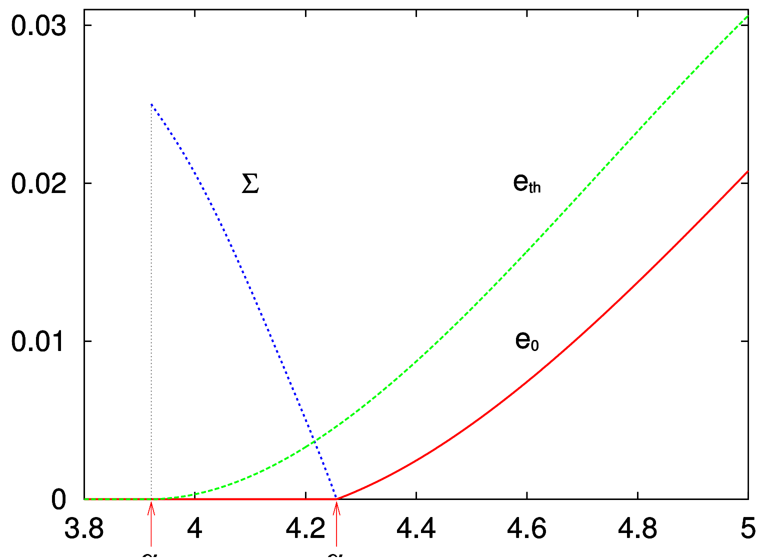
$\eta_{a\to 1}$: known exactly from joint probability of incoming warnings.

SP approximation: this joint probability factorizes

Thermodynamics and complexity

Qualitative behaviour of the complexity:

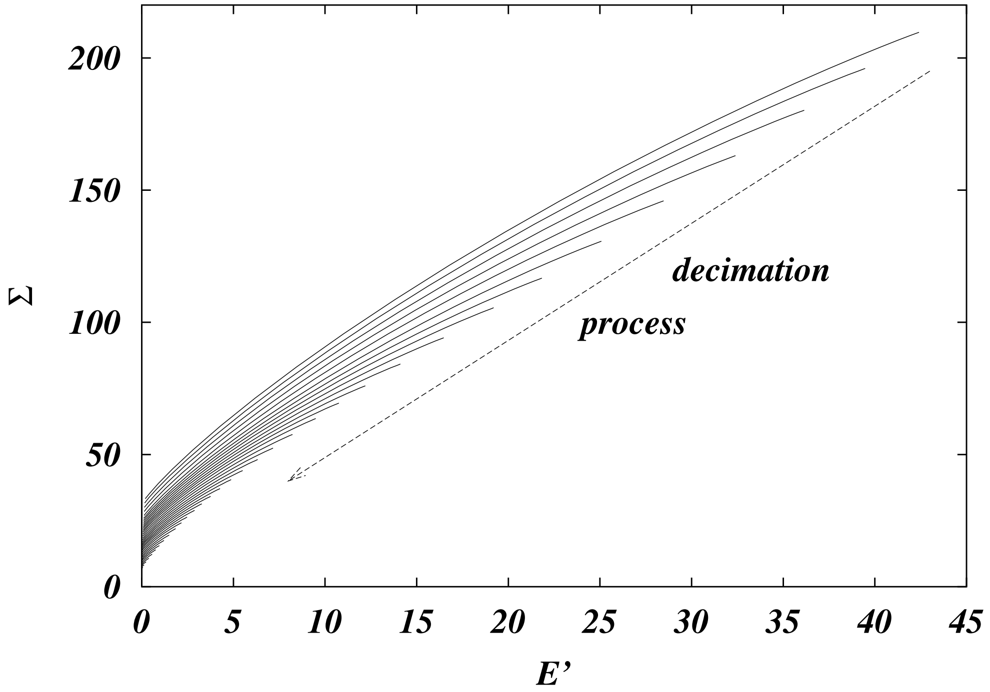




NB: Stability to further sub-clustering: stable in a finite region around α_c.
Conjecture: $\alpha_c = 4.2667...$ is the exact threshold.

Single sample analysis: a new algorithm

Order parameter= Survey of local polarizations, in all states → Algorithm for the Hard-SAT phase. Survey Inspired Decimation: fix the variable which is most biased, rerun the survey propagation, iterate...



Solves typical random 3sat

up to $N = 10^7$ at $\alpha = 4.23$,

complexity $O(N \log N)$.

Local surveys of magnetic fields → a lot of information. Probably possible to invent other algorithms based on the surveys.

Digression 1: unsatisfied glasses

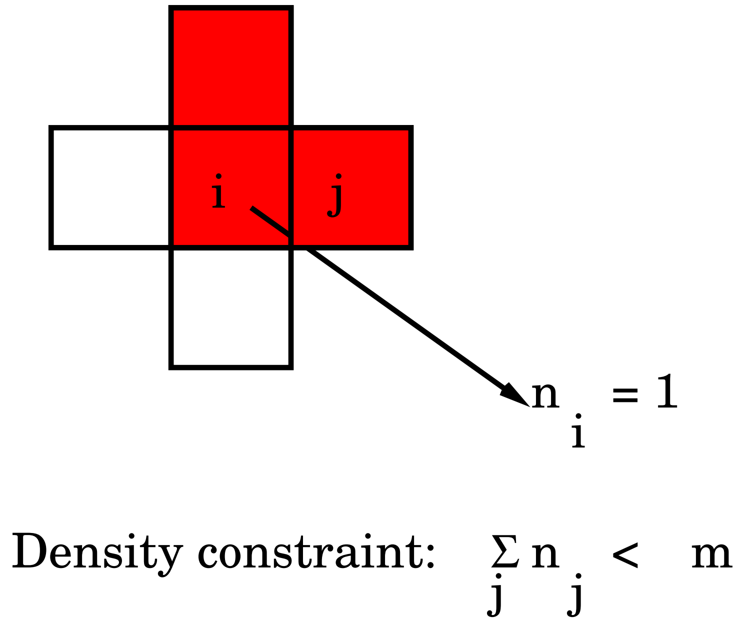
Glass formation in systems with short range repulsion (e.g. hard spheres): geometric frustration. Local densest structure (icosahedral) incompatible with long range crystalline order.

Lattice glass models (Biroli MM, Coniglio et al.,...): density constraint

Same treatment:

dynamical transition at density ρ_d,

static transition at $\rho_c > \rho_d$.

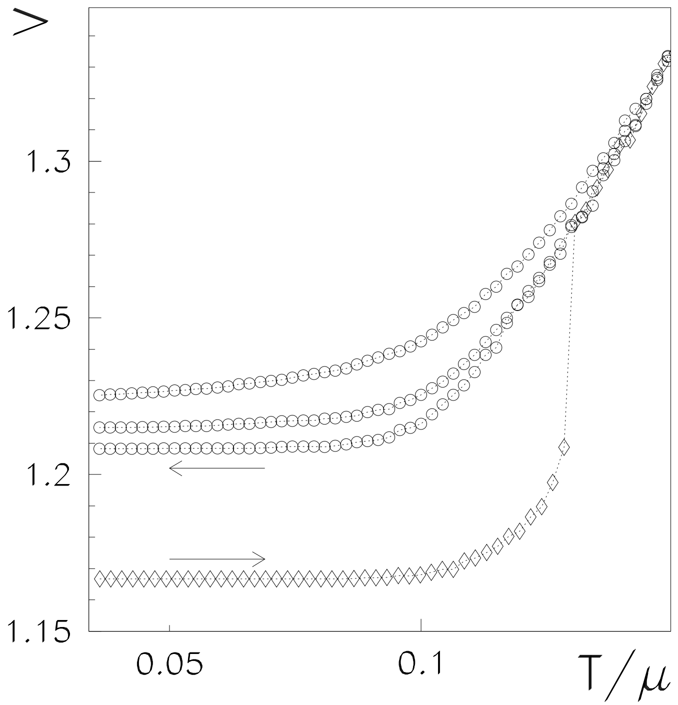


Lattice glasses

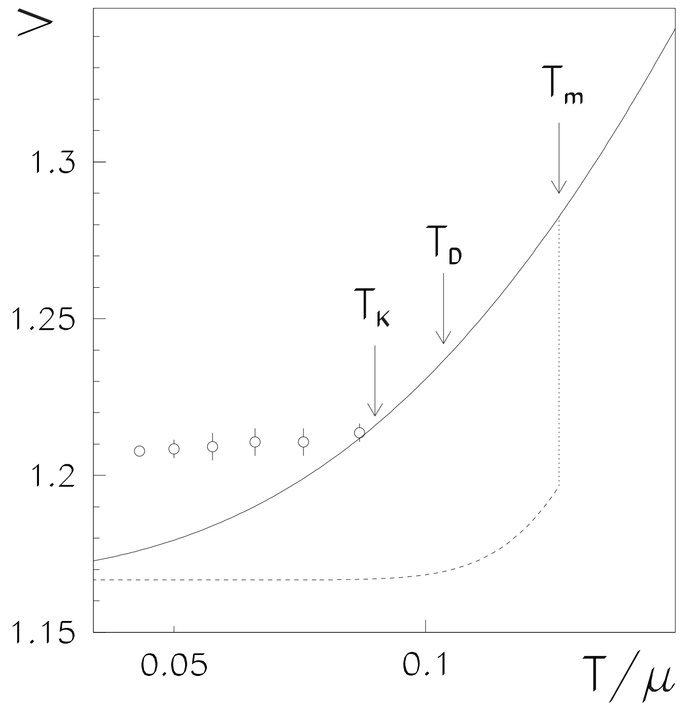
Simulations of related

lattice glass in $d = 3$

(Pica-Ciamarra et al.):



Bethe approximation:



Digression 2: Inference

N discrete variables x_i.

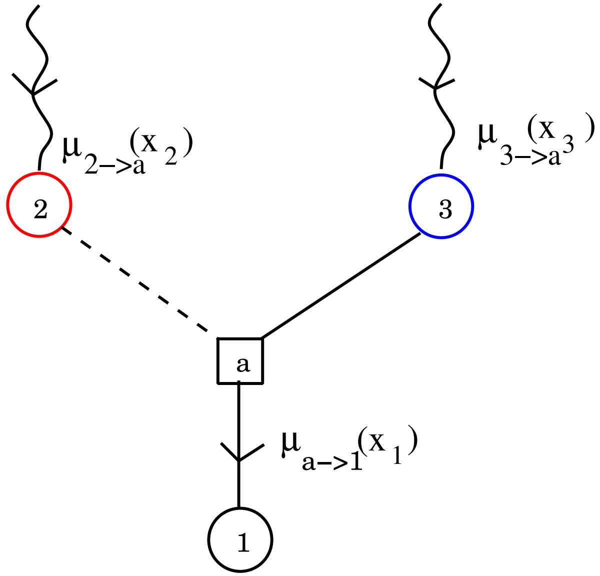
M constraints of probabilistic nature: $\psi_a(X_a)$ = probability of $\{x_{i_1(a)}, ..., x_{i_K(a)}\} = X_a$, according to constraint a, involves K variables.

$P(x_1, ..., x_N) = \prod_{a=1}^{M} \psi_a(X_a)$ Q: Probability of x_i?

Example 1: Medical diagnosis. Variables x_i = Symptoms and diseases. $K = 1, 2$, $\psi_{ij}(x_i, x_j)$ models the statistical dependence between symptom i and disease j; the patient dependent $\psi_i(x_i)$ gives the evidence for symptom i. Compute the probability $p_j(x_j)$ that the patient has disease j.

Other examples: Error correcting code: compute the most likely interpretation of a noisy message. Physics: compute the local magnetization in a set of interacting spins. Optimization: Compute the probability of a variable, given a set of constraints: e.g. graph colouring, or satisfiability...

'Simple' cases of inference: Belief propagation (BP)= Bethe approximation



$\mu_{a\to i}(x_i)$ = Prob(constraint a satisfied), given x_i.
$\mu_{i\to a}(x_i)$ = Prob(var i takes value x_i), when a is absent.

$$\mu_{a\to 1}(x_1) = \sum_{x_2,x_3} \psi_a(x_1,x_2,x_3)\mu_{2\to a}(x_2)\mu_{3\to a}(x_3)$$

$$\mu_{2\to a}(x_2) \propto \prod_{b\in V(2)\setminus a} \mu_{b\to 2}(x_2)$$

Works well for error correcting codes.

Limit of constrained spins $\to$'warning propagation'.

Beyond BP: 1)Small loops $\to$ cluster variational methods 2)Many states $\to$ SP.

Summary

- A fertile emerging field of research at the intersection between computer science, information theory and statistical physics.

- Difficult optimization problems: near to phase transitions, well separated 'clusters' of solutions.... glass phase!

- Analytic result on the generic samples of random 3sat: Phase diagram; Slowdown of algorithms near to $\alpha_c = 4.267$ due to the existence of a Hard SAT phase at $\alpha \in [\sim 3.9, 4.267]$, with exponentially many states.

- Single sample analysis: Survey propagation: a very efficient algorithm for solving random 3sat problems. Applicable to many "constraint satisfaction problems". An application for 'useless' spin glasses :-)

Collaborators

- G. Parisi (Univ. Roma 1), R. Zecchina (ICTP Trieste)

- A. Braunstein (Trieste), S. Ciliberti (Madrid),O. Martin (Orsay), S. Mertens (Magdeburg), F. Ricci-Tersenghi (Roma), O. Rivoire (Orsay), M. Weigt (Göttingen).

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