Can Nature solve hard problems?

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Nature and hard problems

- "Hard problems": discrete optimization (combinatorial)
- Nature. Designed experimental devices, "nature-inspired" algorithms.... Classical

    - A different topic: Nature poses complicated problems (chemistry, strings, consciousness,...)

Combinatorial optimization problems

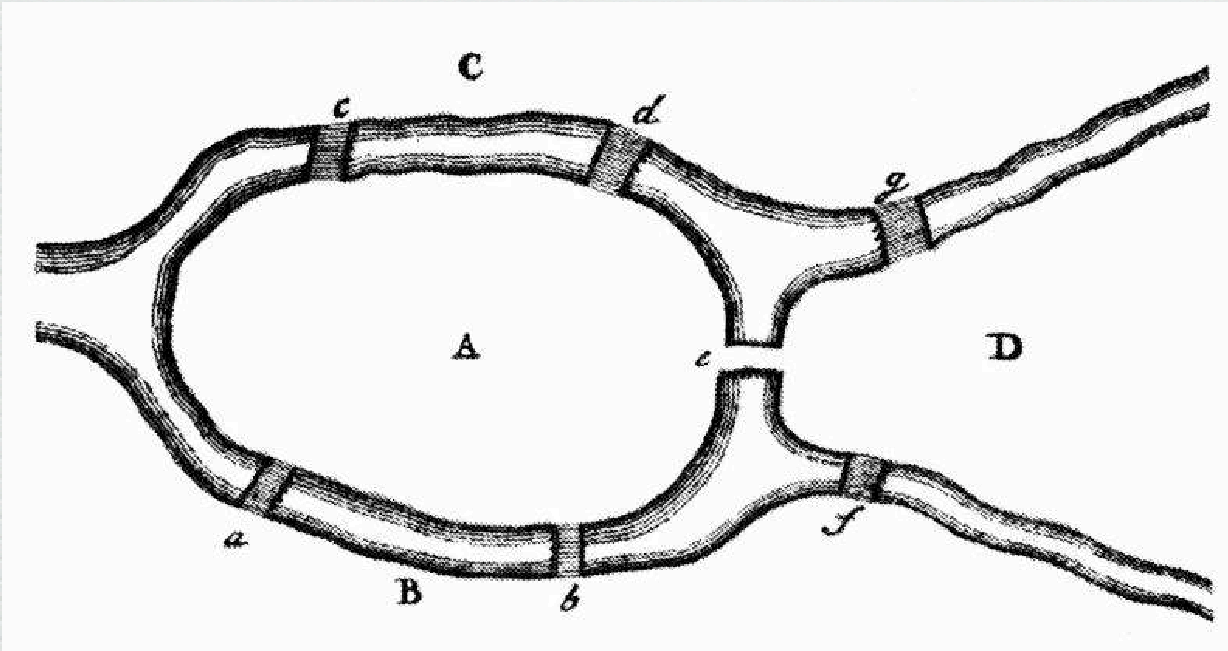
- many simple variables $x = (x_1, \cdots x_N), \; N \gg 1$
- Cost function $E(x)$, computable in $O(N^b)$ operations
- Find configuration of lowest cost

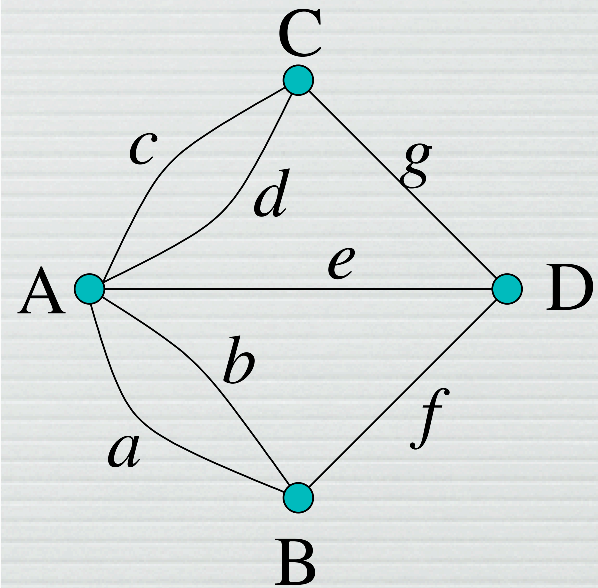
Examples: Travelling Salesman Problem, Eulerian circuit, Hamiltonian circuit, Spin Glasses, Satisfiability, Random Field Ising Model, Protein folding, ...

Many applications, in computer science, physics, information theory $\longrightarrow$ chip design, schools, airlines, etc...

Eulerian circuit

Königsberg seven bridges





Euler, 1736:

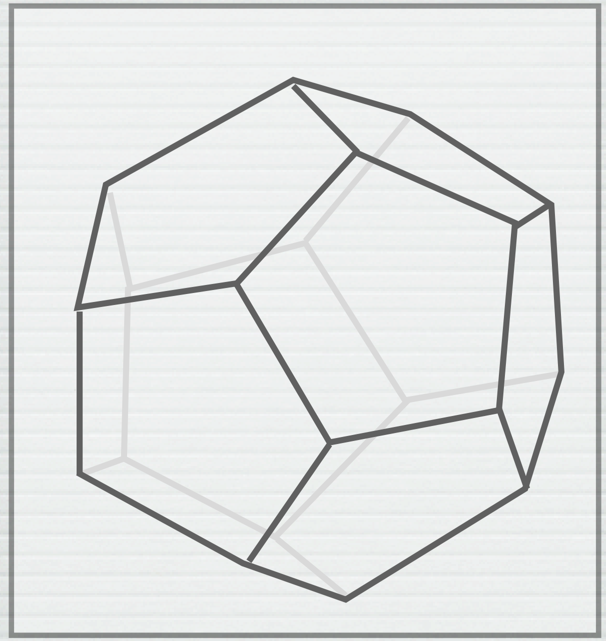
SOLVTIO PROBLEMATIS
AD
GEOMETRIAM SITVS
PERTINENTIS.
AVCTORE
Leonh. Eulero.

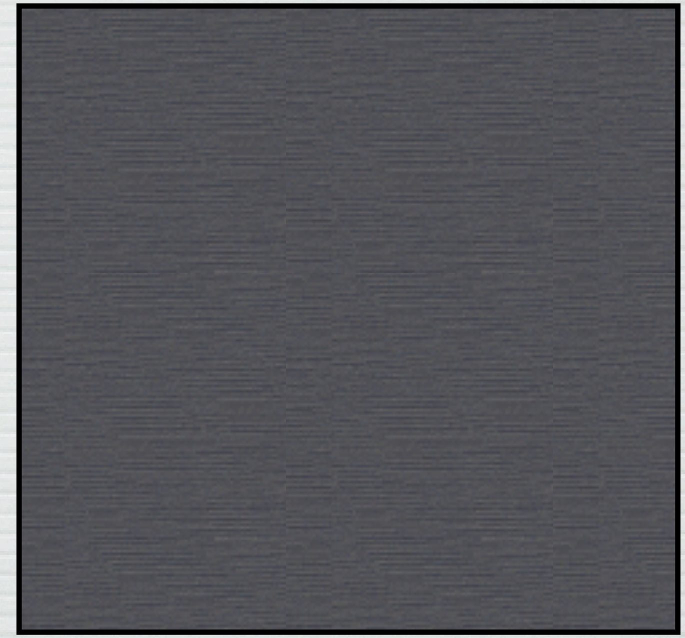
Graph, visit all edges exactly once

“Eulerian circuit” ⟷ every vertex has even degree

Hamiltonian circuit

Hamilton's
"Icosian game"





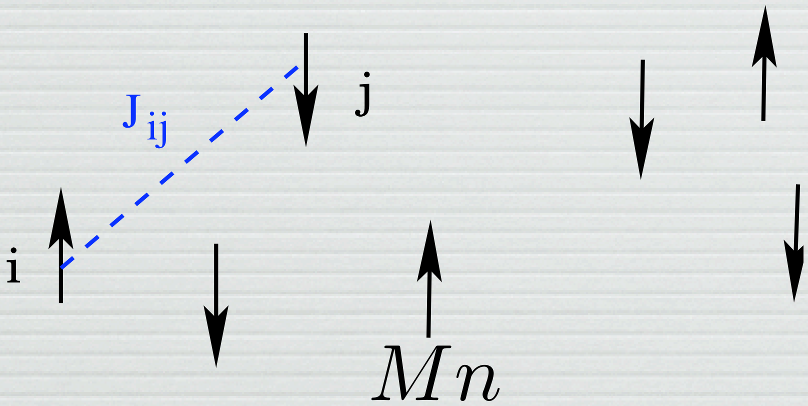
Sir William, Astronomer Royal of Ireland, 1859

Graph, visit all vertices exactly once
No simple algorithm!

Spin glasses

- Many atoms, microscopic interactions are known, "disordered systems"

e.g.: CuMn



$\sigma_i = 1$

$\sigma_i = -1$

$$E = -\sum_{ij} J_{ij}\sigma_i\sigma_j$$

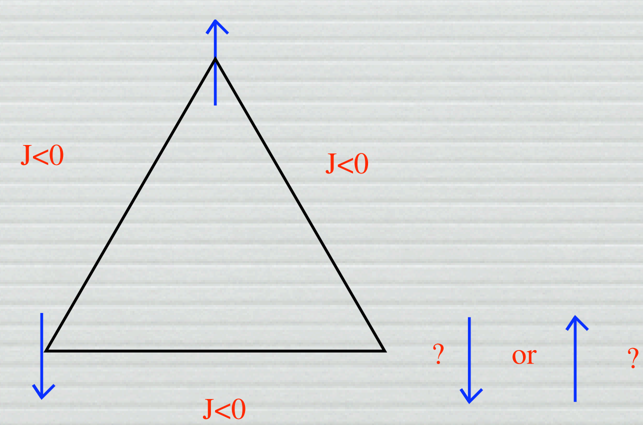
$$P_T(\sigma_1, .., \sigma_N) = \frac{1}{Z}\exp\left(\frac{1}{T}\sum_{ij} J_{ij}\sigma_i\sigma_j\right)$$

➡ Each spin 'sees' a different local field

➡ Low temperature: frustration

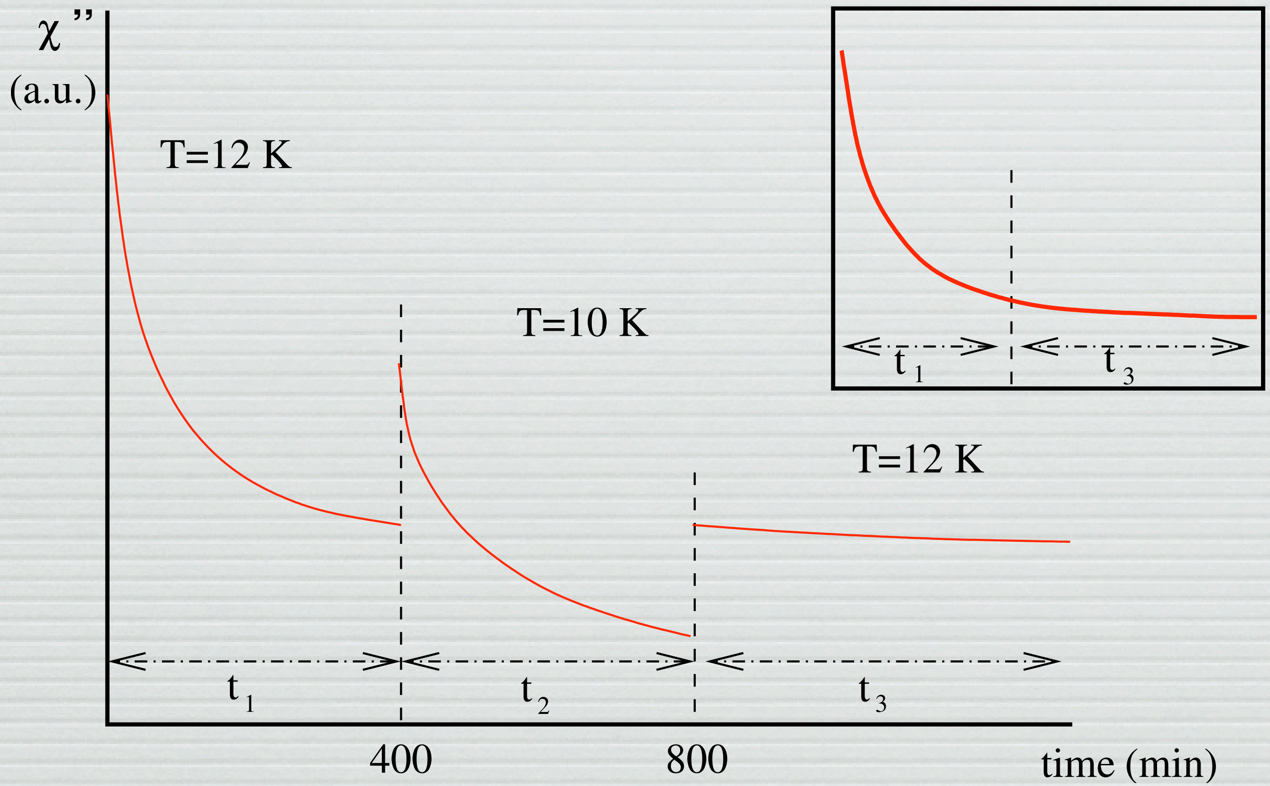
➡ Spins freeze in random directions

➡ Difficult to find min. of E



Useless, but thousands of papers...

Spin glass experiment: relaxation of magnetic susceptibility



Slow dynamics
Aging
Memory

Ultrametricity=
Hierarchical
structure of
metastable states

E. Vincent et al, SPEC

What are the hard problems?

N discrete variables, energy= sum of many terms...

Question: Does there exist a configuration of energy < A?

P= Polynomial, $t = O(N^c)$

Ex: Assignment, Eulerian circuit, Spin glass in d=2 ...

NP= "Non deterministic polynomial",

A "yes" answer can be checked in $t = O(N^c)$

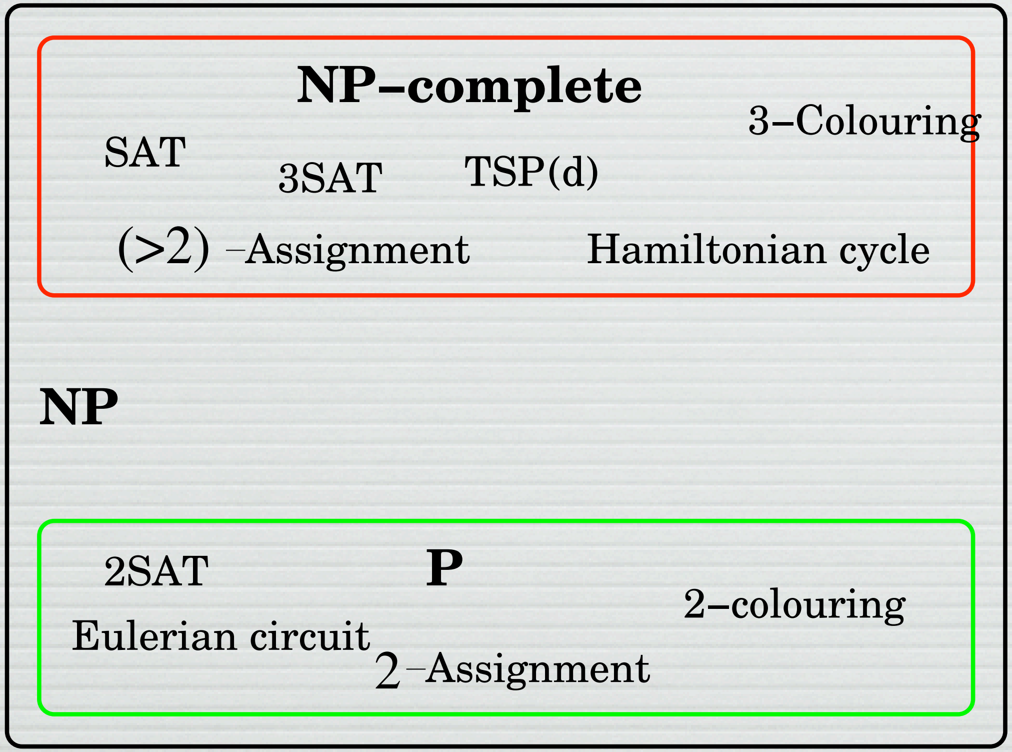
Many problems!

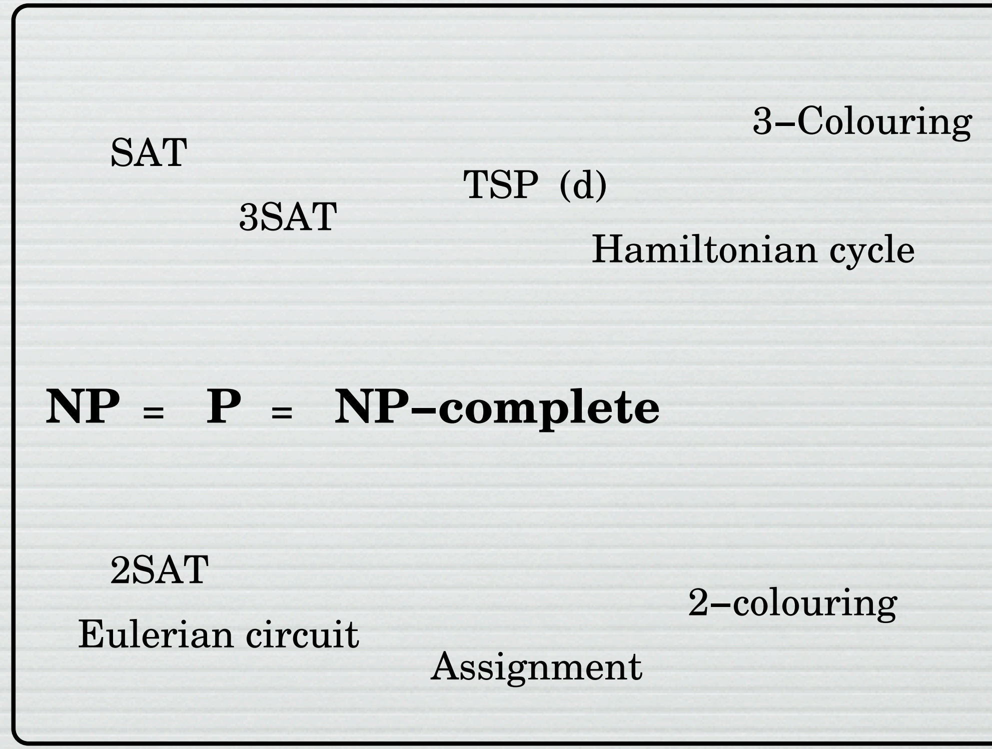
NPC = The hardest in NP: a problem is NPC iff all problems in NP can be mapped to it in polynomial time

Th (Cook 71): Satisfiability is NPC

Many others: Hamiltonian circuit, Spin glass in d=3, Steiner trees, Travelling salesman...

What are hard problems?





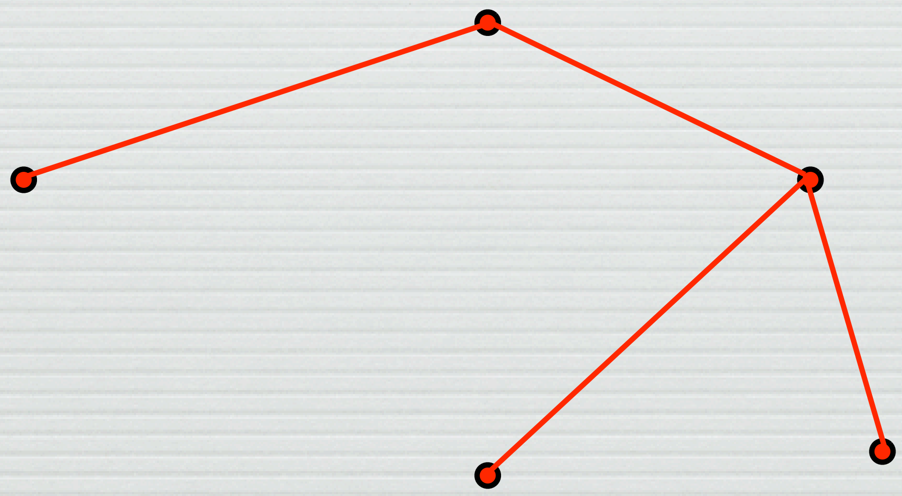
Conjectured

Possible

Is P different from NP?

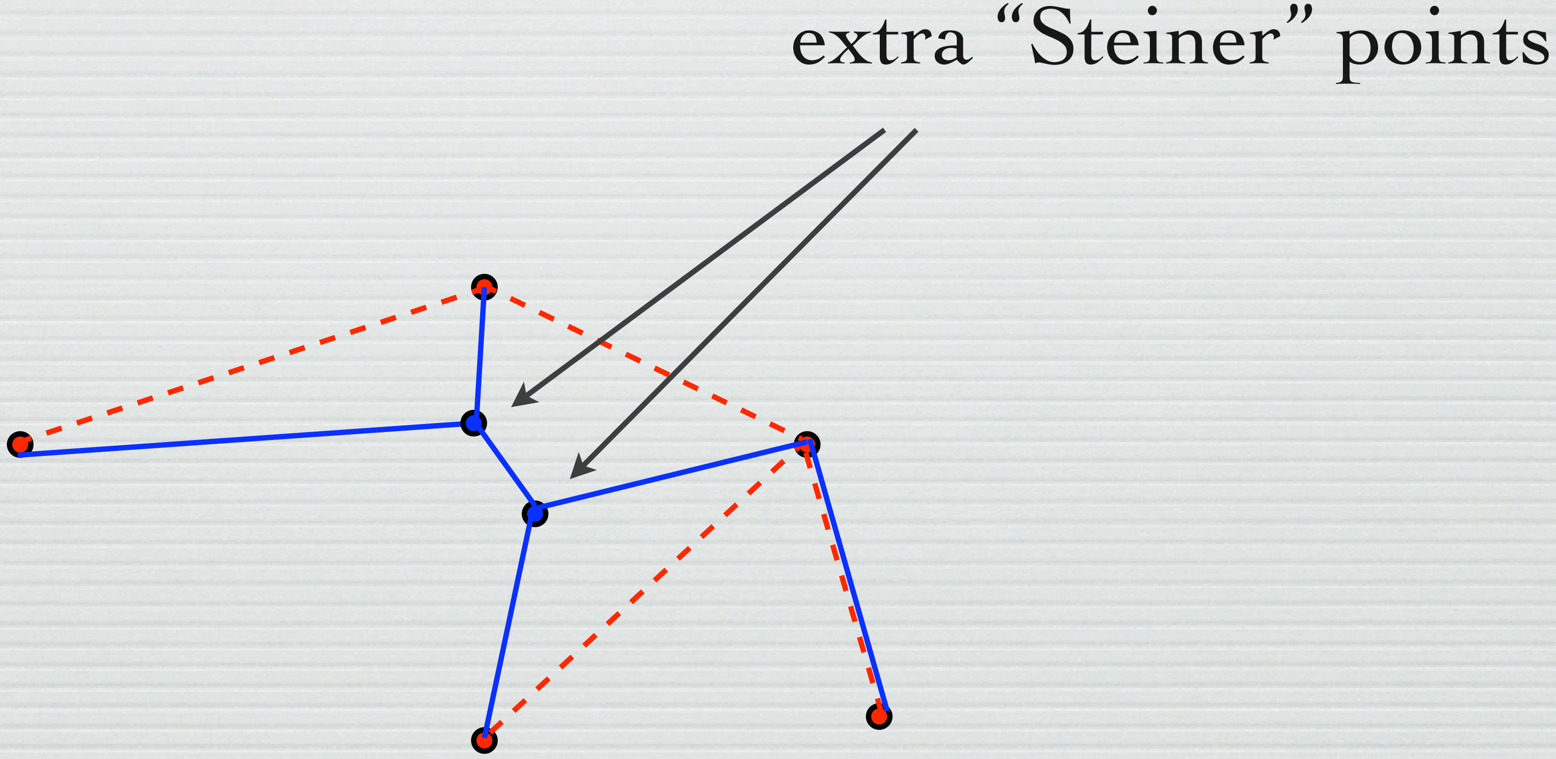
NB: worst case analysis

Physics and hard problem: the example of Steiner trees



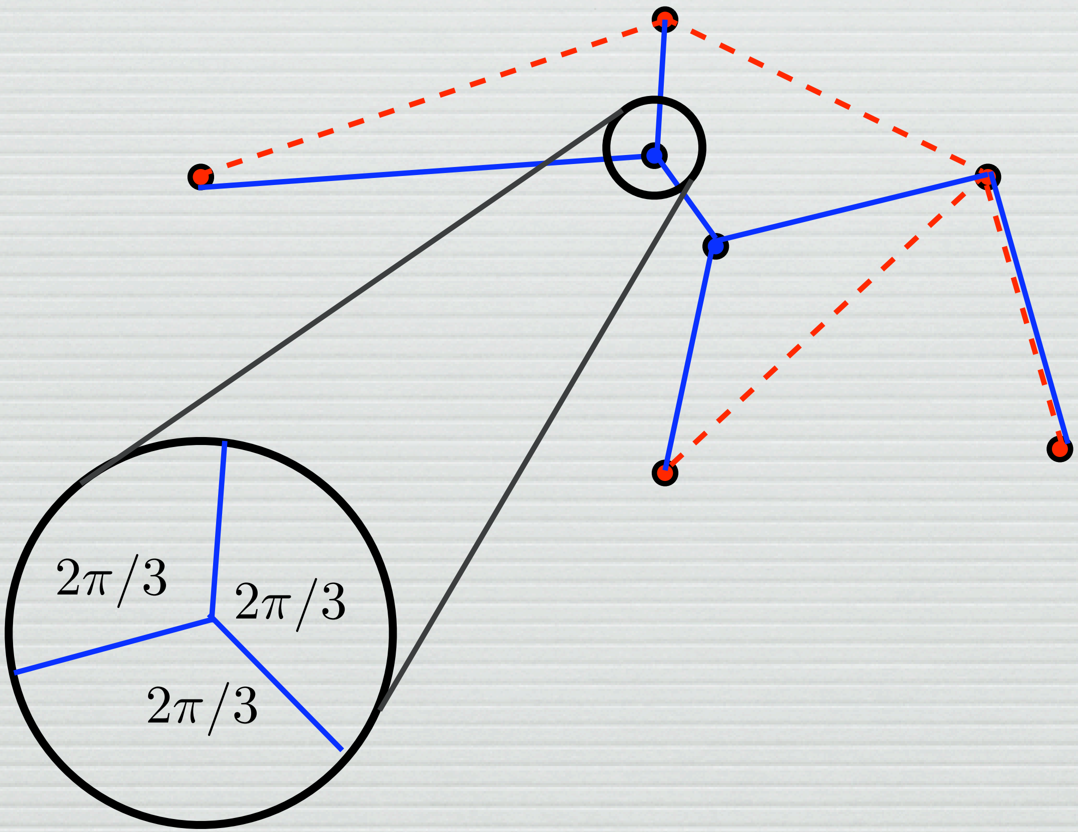
N points in the plane.
Find the tree with minimal length joining them
NP-complete

Steiner trees



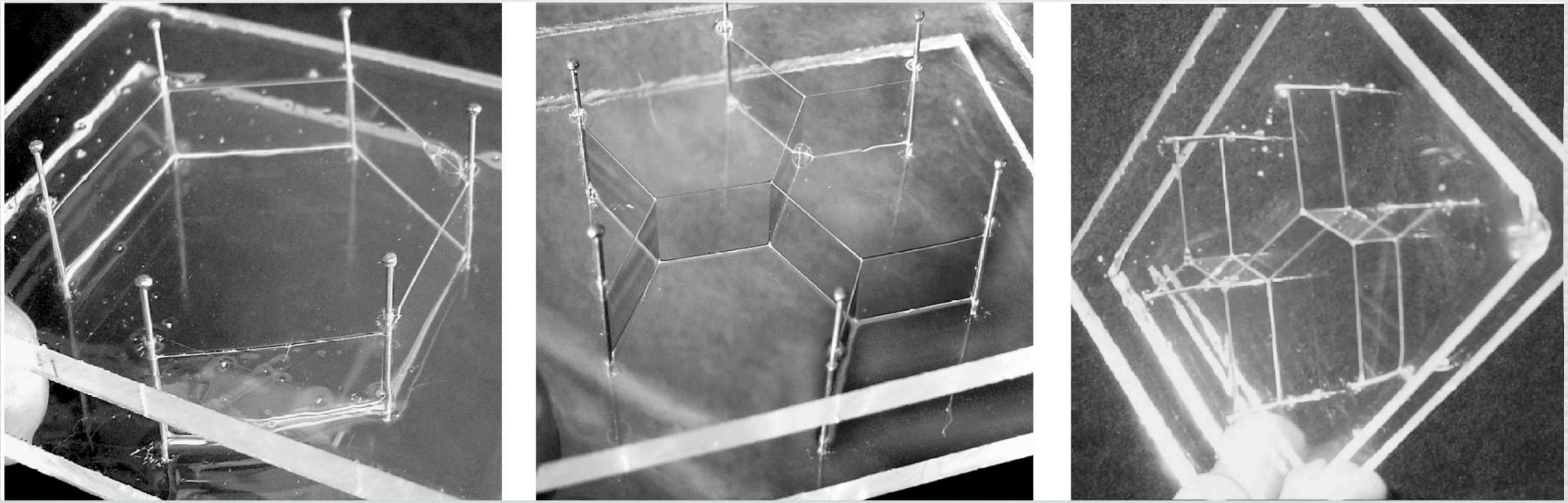
Steiner trees

Minimal length= constant cohesive force
Local equilibrium



A first example: Steiner trees

Physical realization: soap films in two dimensions

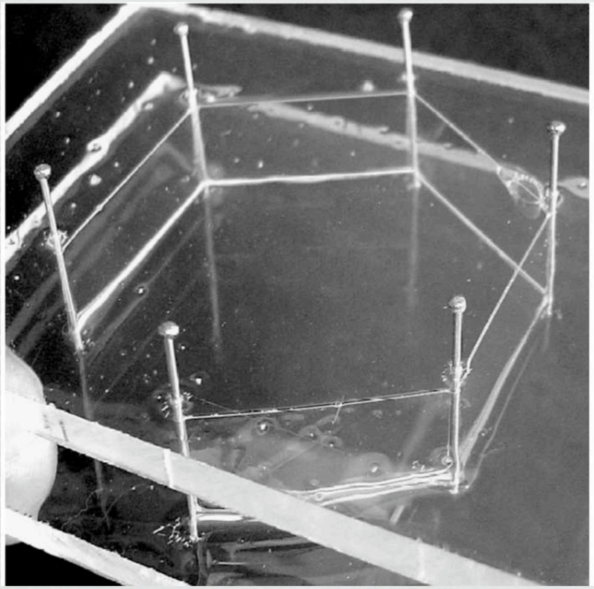


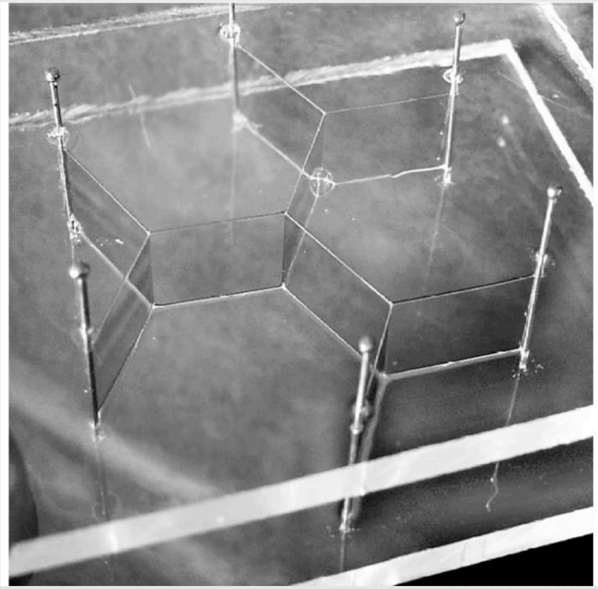
Duttal, Khastgir and Roy 2008

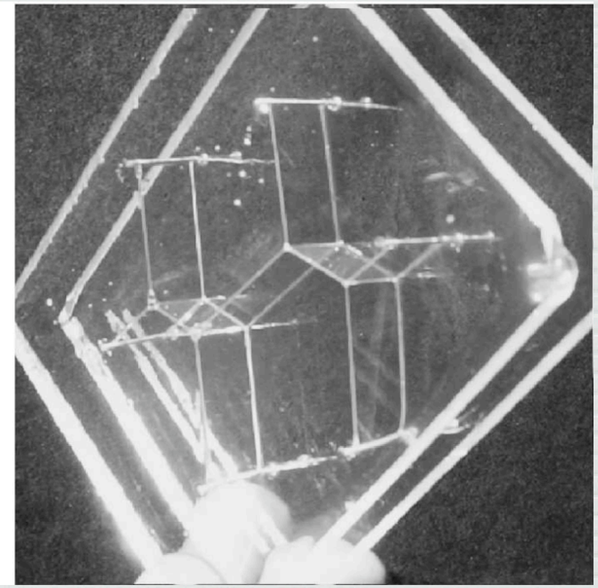
Soap film: energy E proportional to the area
Film between two parallel plates: E prop. to length

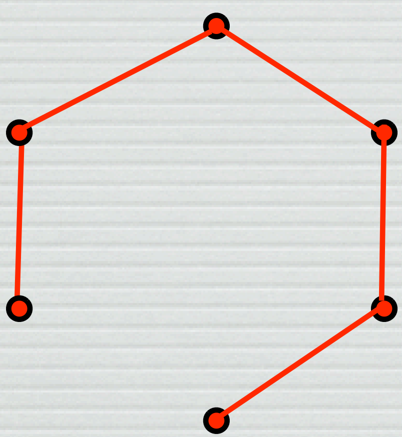
Optimal tree

Metastable states

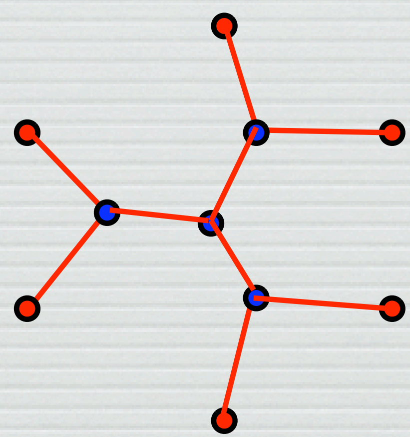




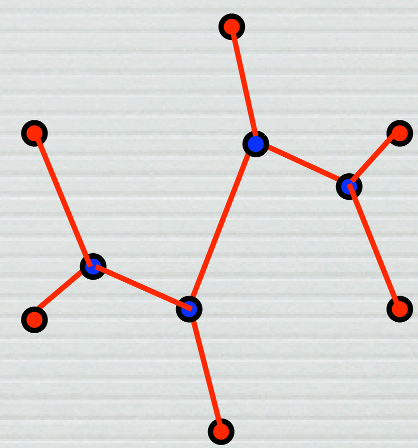




$L = 5$



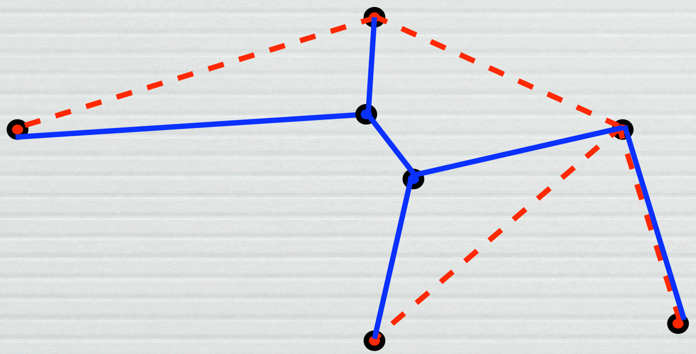
$L = \sqrt{27}$



$L = \sqrt{28}$

Steiner trees and metastability

- Local equilibrium once topology is fixed: OK
- Global search of topologies: $\sim 2^{cN}$ possibilities



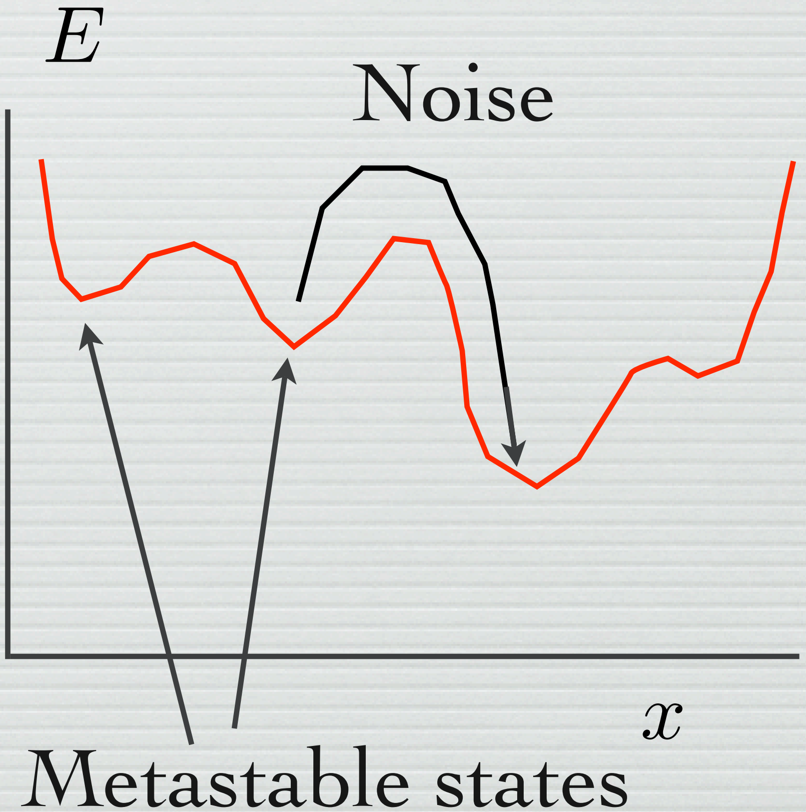
Macroscopic system $\longrightarrow$ huge energy barriers to reach the optimal -minimal energy- state

No quantum tunneling
No thermal hopping } on human time scale

Natural "thermal" way out of metastability

Smaller scales (or computer implementation) + thermal noise.

- Programming a large problem: physical design problem... or physics inspired simulations
- Noise often helps to jump over some barriers: simulated annealing (Kirkpatrick et al 1983)

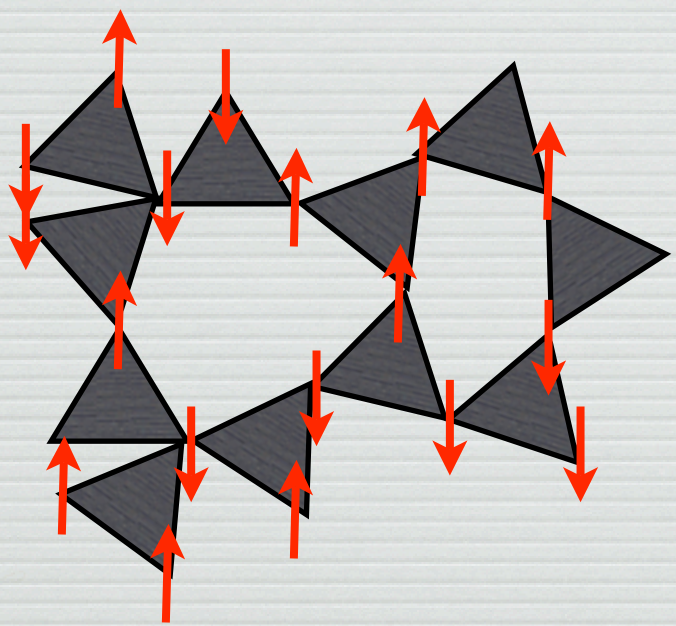


- "Glassy" systems with collective barriers: never equilibrate

Trapped in a glass phase

Structural glasses, spin glasses, electron glasses, vortex glasses... never reach their lowest energy state

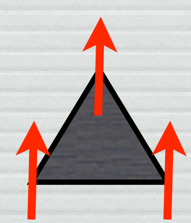
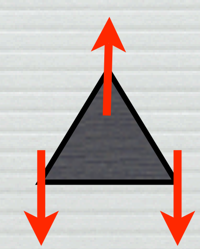
Spin glass model:
3-spin interaction



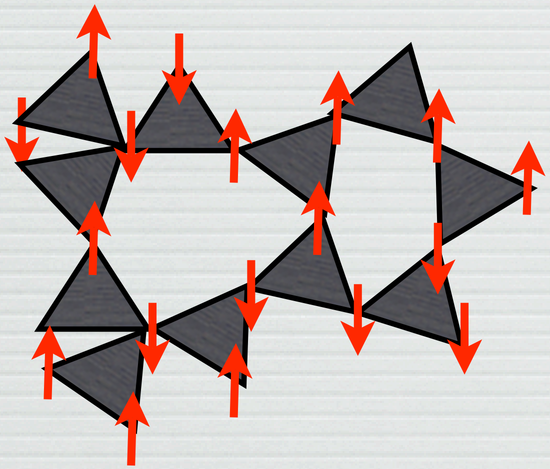
 $s_i = 1$

 $s_i = -1$

$$E = -\sum_{ijk} s_i s_j s_k$$

 or  or...

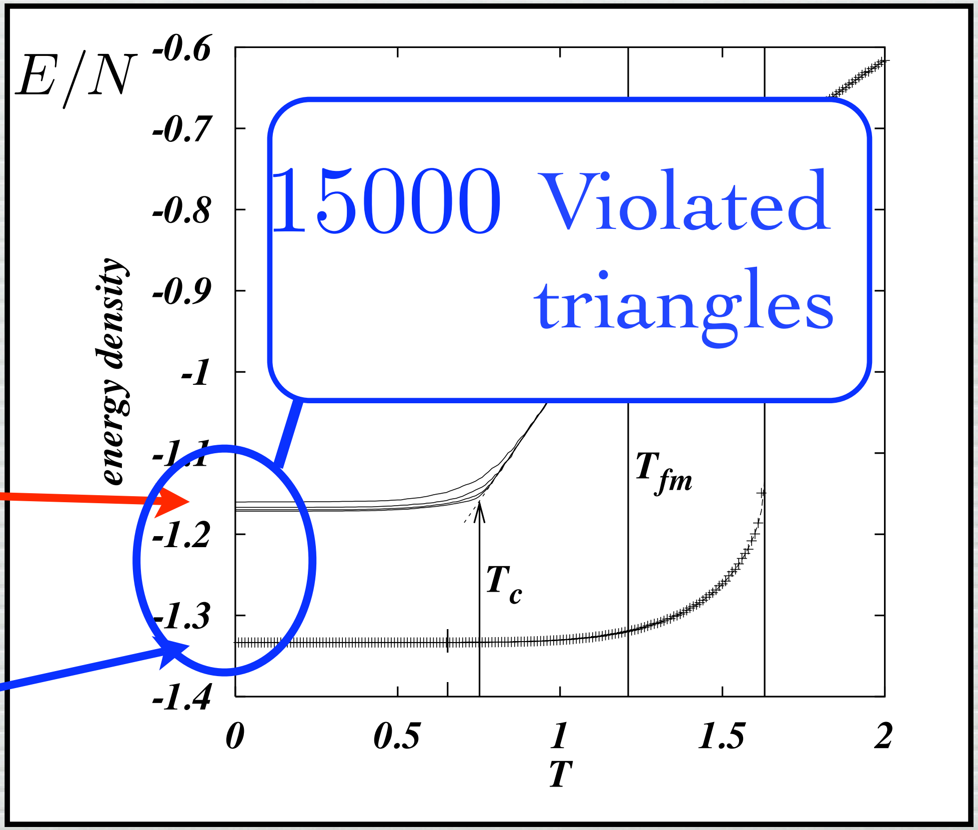
Trapped in a glass phase



$$E = -\sum_{ijk} s_i s_j s_k$$

10^5 spins, 4 triangles per spin

Metastable states found by simulated annealing 10^4 to 10^7 steps



Optimal state, all $s_i = 1$

Random first order phase transition at T_c : traps

Non "thermal" ways out of metastability

"Glassy" systems with random first order transition:
- very difficult to equilibrate with thermal methods
- subtle memory effects

- (Generate all states in parallel -e.g. DNA computing-, and select. Soon facing atomic resolution)
- (Genetic algorithms)
- ...
- Message passing algorithms for constraint satisfaction problems.

A large class of problems: graphical models

$$P(x_1, ..., x_N) = C \prod_{a=1}^{M} \psi_a(X_a)$$

$$X_a = \{x_{i_1(a)}, \cdots, x_{i_K(a)}\}$$

- Satisfiability of Boolean formulas
- Steiner tree in a graph
- Graph coloring
- Decoding in error correcting codes
- Group testing
- Spin glasses
- Learning in neural networks
- ....

Satisfiability

"..a theatrical director feels obligated to cast either his ingénue, Actress Alvarez, or his nephew, Actor Cohen, in a production. But Miss Alvarez won't be in a play with Cohen (her former lover), and she demands that the cast include her new flame, Actor Davenport. The producer, with her own favors to repay, insists that Actor Branislavsky have a part. But Branislavsky won't be in any play with Miss Alvarez or Davenport.[] Is it possible to satisfy the tangled web of conflicting demands?"

(from G. Johnson, The New York Times 1999).

$$A, B, C, D \in \{0, 1\}$$

Constraints = clauses, e.g.: $A \vee C$

Satisfiability: an important problem

N Boolean variables, M constraints (clauses)

$$x_1 \vee x_{27} \vee \bar{x}_3, \quad \bar{x}_{11} \vee x_2, \; ....$$

Can one fix the values of the variables to T(=1) or F(=0) such that all the constraints are satisfied?
Uniform measure over all solutions:

$$P(x_1, \cdots, x_N) = \frac{1}{Z} \, \mathbb{I}\big((x_1, x_{27}, x_3) \neq (0,0,1)\big) \, \mathbb{I}\big((x_{11}, x_2) \neq (1,0)\big) \, \cdots$$

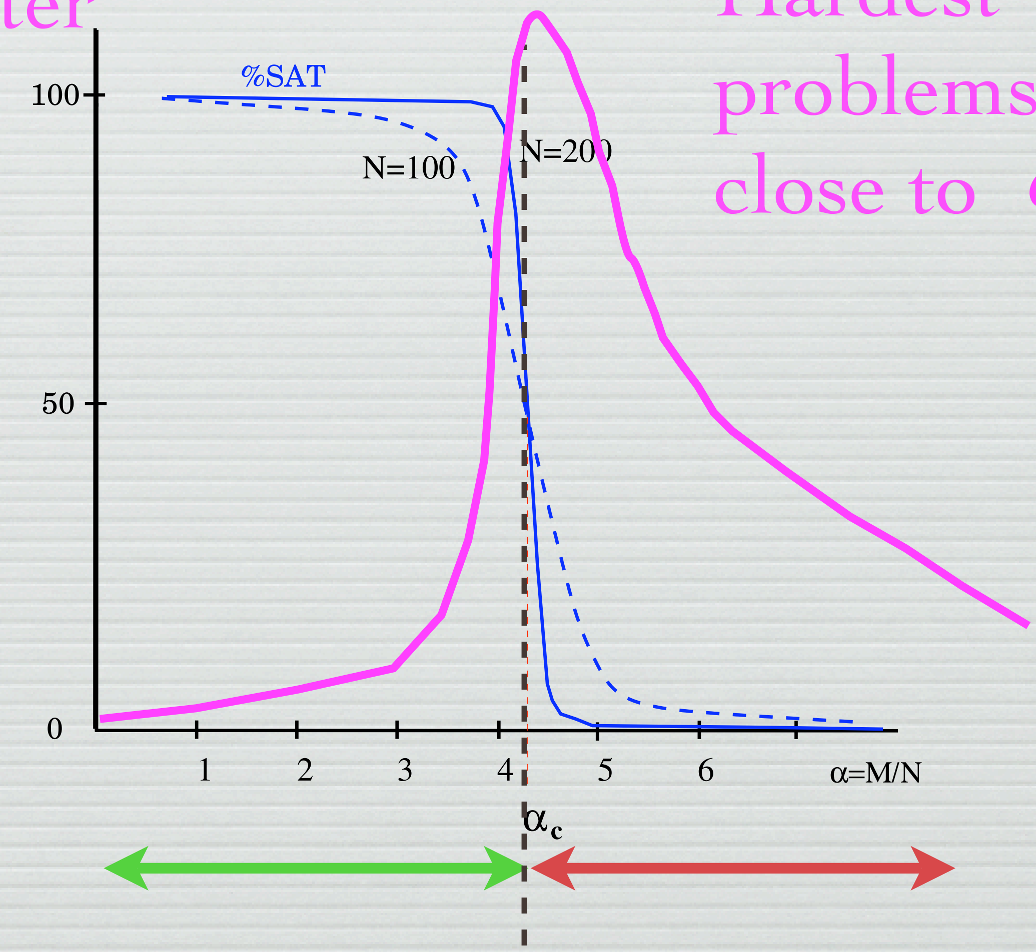
The “grandfather” of NP complete problems.
Conjunctive normal form for logical formulae.

Typical satisfiability and phase transition

Random 3-SAT: N variables. 3 variables in each clause, randomly chosen among N, randomly negated:

Large N limit:

Computer time



Hardest problems: close to α_c

SAT for $\alpha < \alpha_c$

UNSAT for $\alpha > \alpha_c$

“Phase transition”

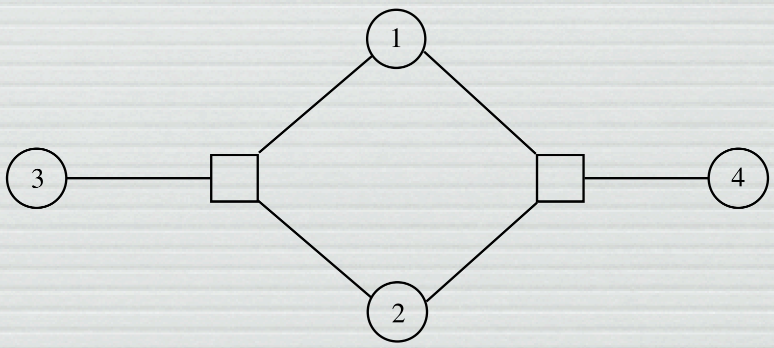
Selman, Kirkpatrick,...

Message passing algorithms

$$P(x_1, ..., x_N) = C \prod_{a=1}^{M} \psi_a(X_a)$$

- Represent interactions in P by a "factor graph"
- Exchange probabilistic messages along the edges of this graph

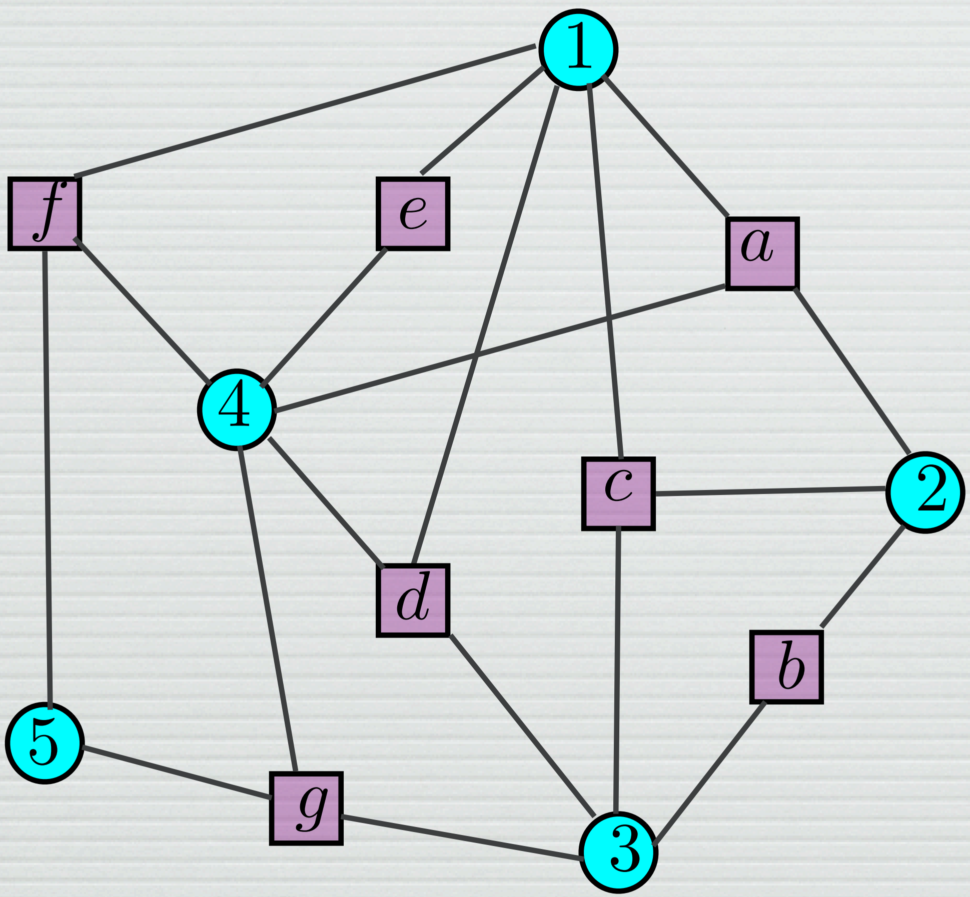
One circle per variable, one square per constraint:



Satisfiability:

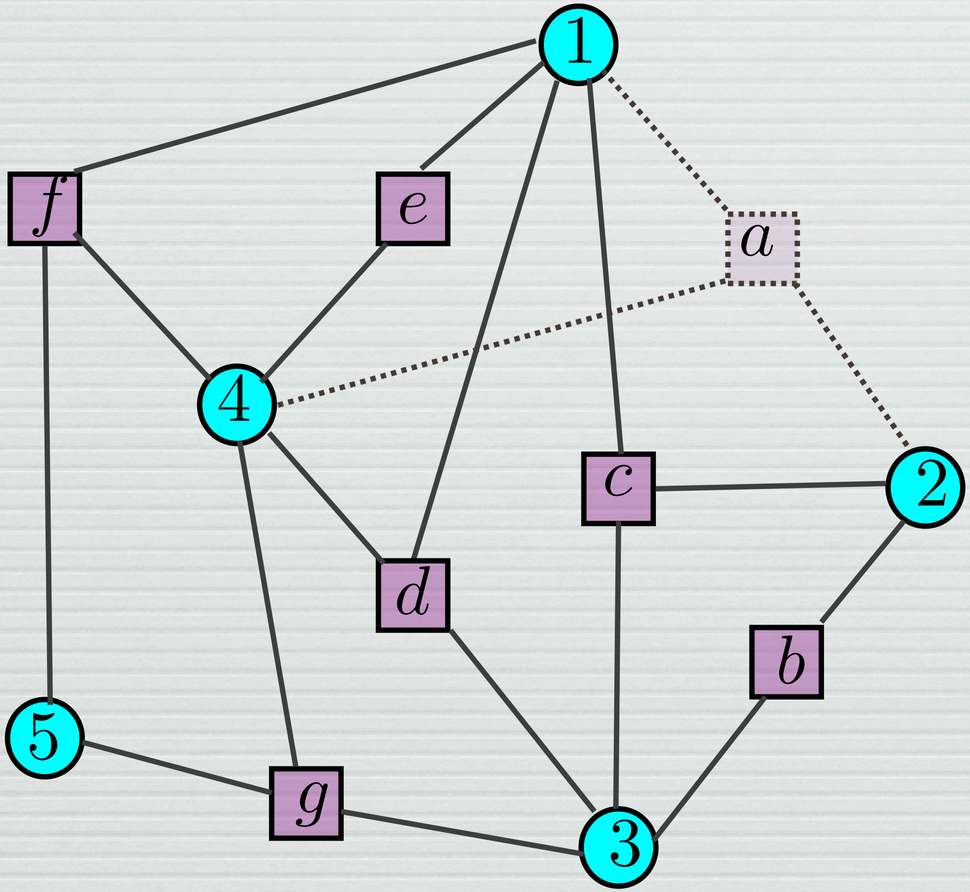
$$(x_1 \vee \overline{x}_2 \vee x_3) \wedge (x_1 \vee \overline{x}_2 \vee \overline{x}_4)$$

Factor Graph



$$P(x_1, \cdots, x_5) = \psi_a(x_1, x_2, x_4)\psi_b(x_2, x_3) \cdots$$

Belief Propagation (cavity equations)

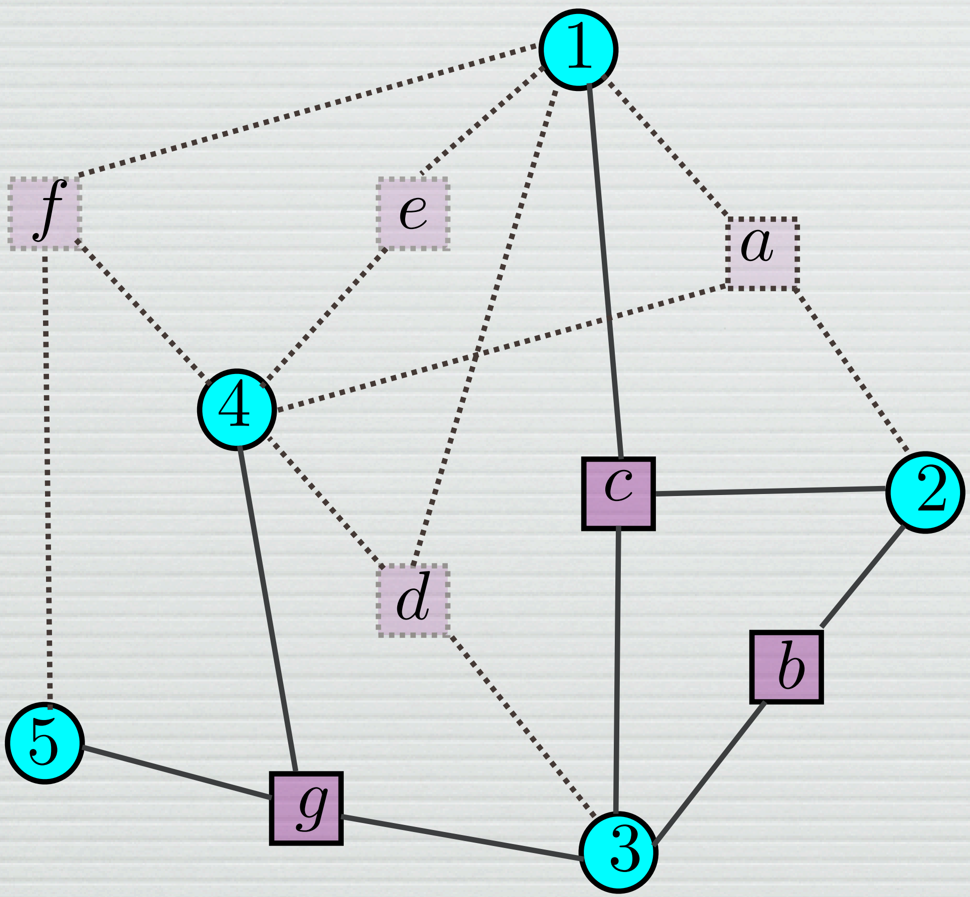


Messages:

Probability of x_1 in the absence of a:

$$m_{1\to a}(x_1)$$

Belief Propagation (cavity equations)

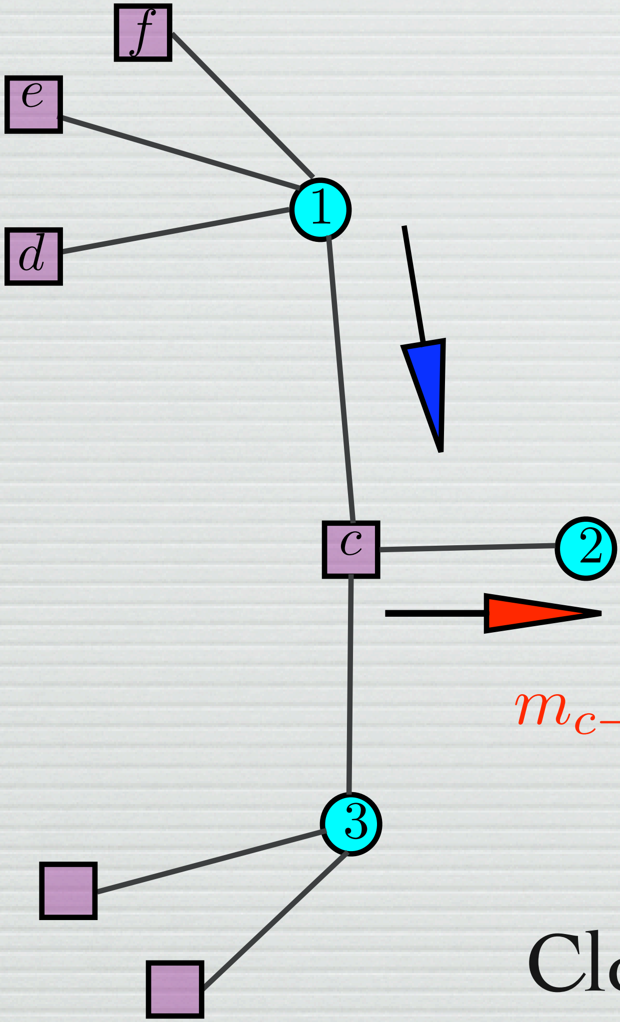


Messages:

Probability of x_1 when it is connected only to c :

$$m_{c\to 1}(x_1)$$

Belief Propagation (Bethe-Peierls, TAP, Gallager, Pearl, cavity equations)

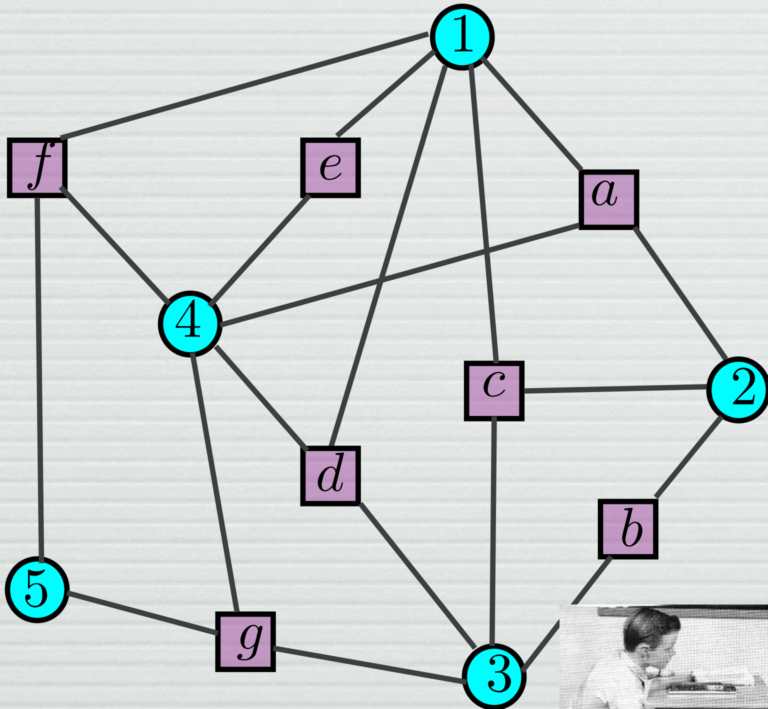


$$m_{1\to c}(x_1) = C m_{d\to 1}(x_1) m_{e\to 1}(x_1) m_{f\to 1}(x_1)$$

$$m_{c\to 2}(x_2) = \sum_{x_1, x_3} \psi_c(x_1, x_2, x_3) m_{1\to c}(x_1) m_{3\to c}(x_3)$$

Closed set of equations: two messages "propagate" on each edge of the factor graph.

Belief Propagation

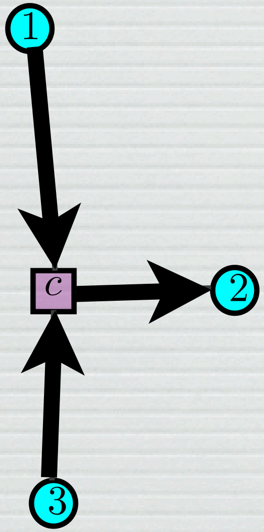


Propagate messages along the edges, update messages at vertices, using elementary local probabilistic rules

"Mean field" type approximation: neglects correlations between variables in the cavity graph.

Improvements: Generalized BP, Survey Propagation

The limits of Belief Propagation



$$m_{c\to 2}(x_2) = \sum_{x_1,x_3} \psi_c(x_1,x_2,x_3) m_{1\to c}(x_1) m_{3\to c}(x_3)$$

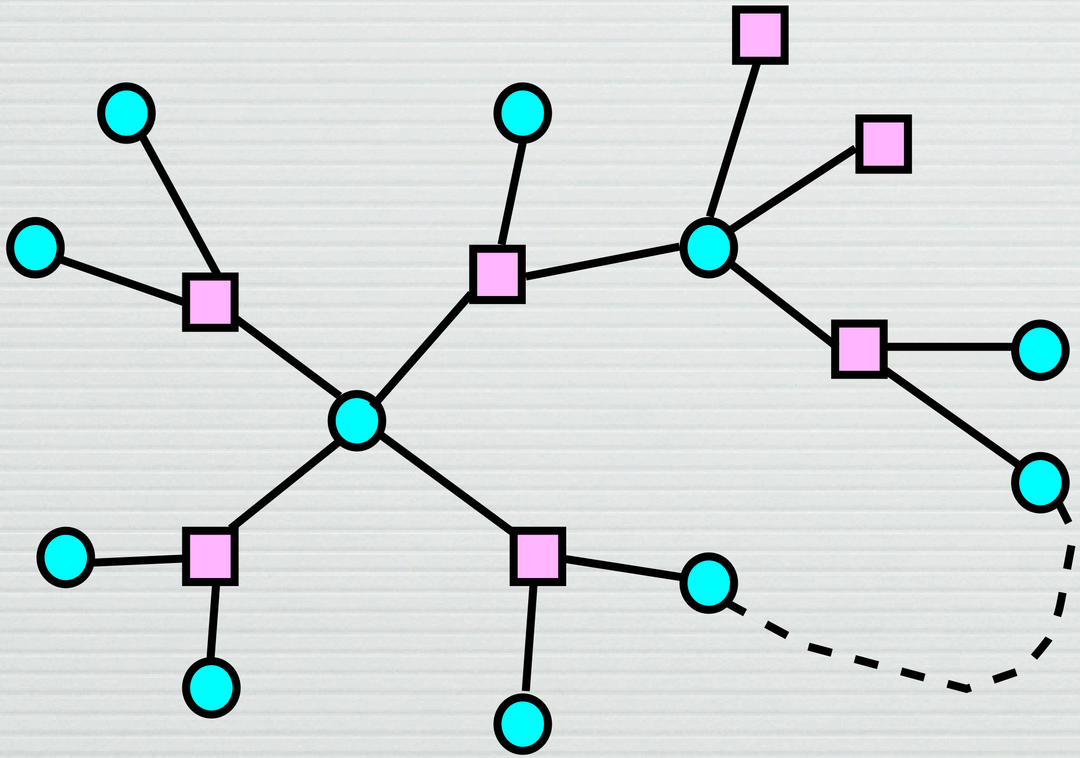
Approximation: independence of x_1 and x_3 in the absence of constraint c :

$$P^{(c)}(x_1,x_3) \simeq m_{c\to 1}(x_1) m_{c\to 3}(x_3)$$

"Mean field" type approximation: neglects correlations between variables in the cavity graph.

Exact on trees, or "locally-tree-like" graphs with correlation decay

Locally-tree-like graphs



Loops: length $O(\log N)$ (e.g. error-correcting codes)

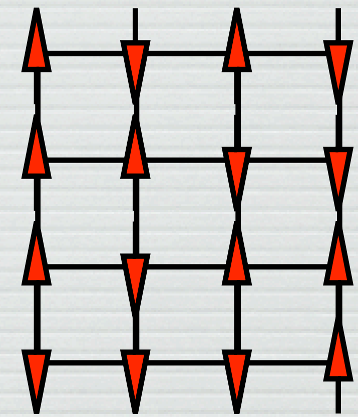
If correlations decay fast enough: BP is OK

Small structures: collective variables (generalized BP)

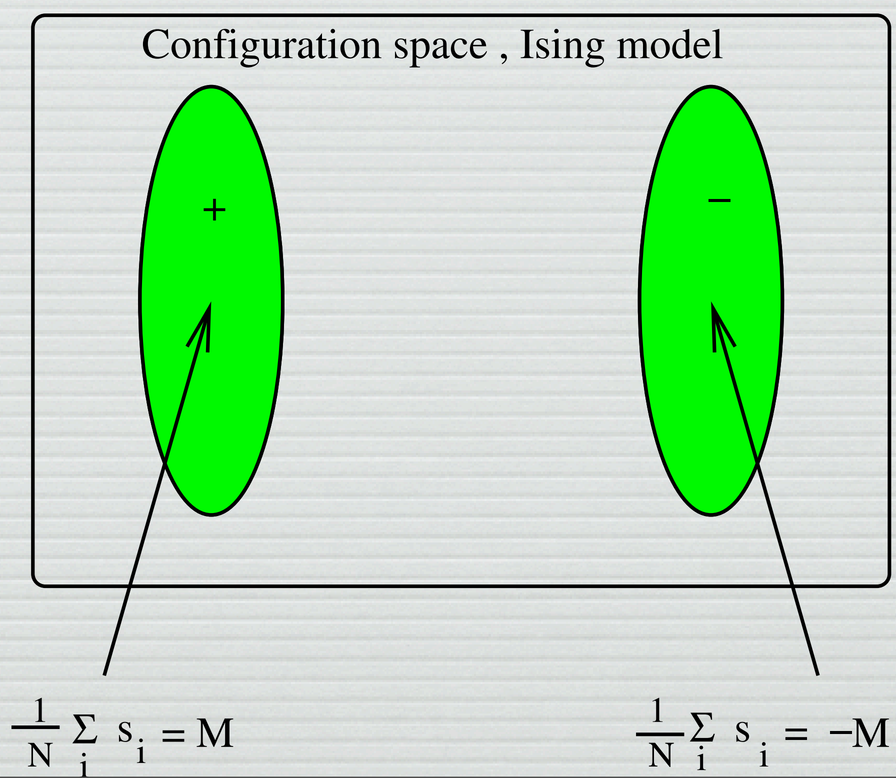
Decay of correlations: non-trivial

$$P^{(c)}(x_1, x_3) \simeq m_{c\to 1}(x_1) m_{c\to 3}(x_3)$$

Holds if the measure is restricted to one cluster (=pure state) of solutions. e.g. Ising model:

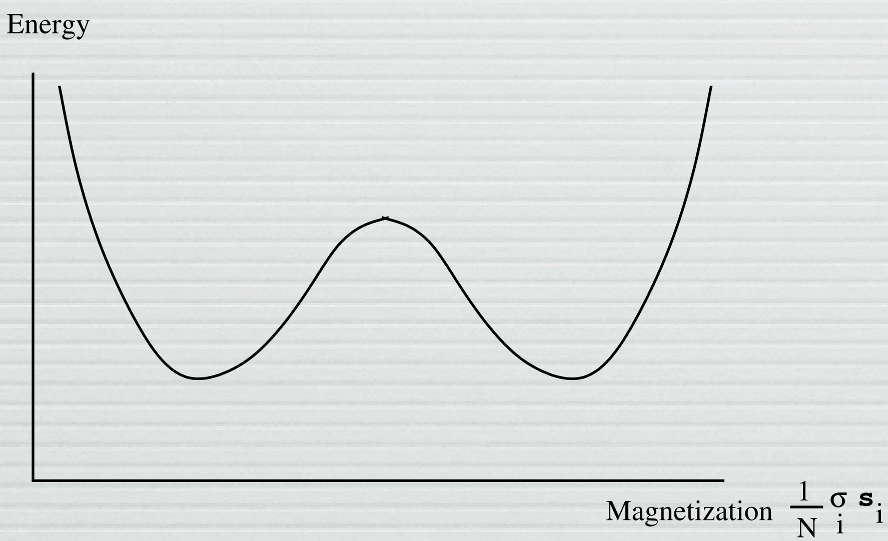


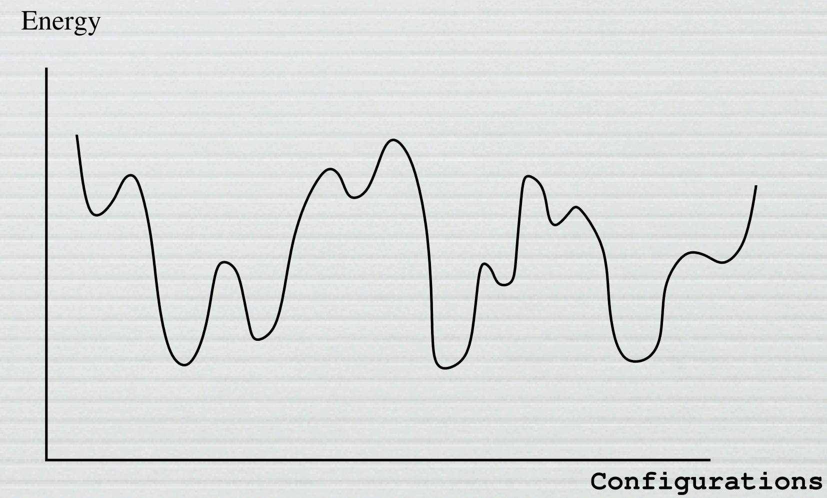
Two states. Correlations decay within one state.



$$P^{(c)}(x_1, x_3) \simeq m_{c\to 1}(x_1) m_{c\to 3}(x_3)$$

Holds if the measure is restricted to one cluster of solutions
One BP solution per cluster. Landscape cartoon:





Ising: two states, two solutions of BP

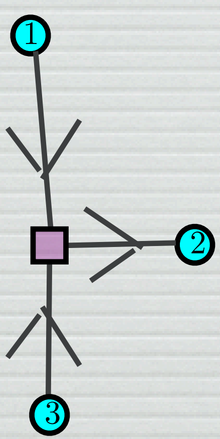
Glassy phase: many states, many solutions of BP

Survey Propagation (SP) = statistics over all solutions of BP. Extremely powerful in a glass phase

Power of message passing algorithms

Approximate solution of very hard, and very large constraint satisfaction problems, ...FAST! (typically linear time)

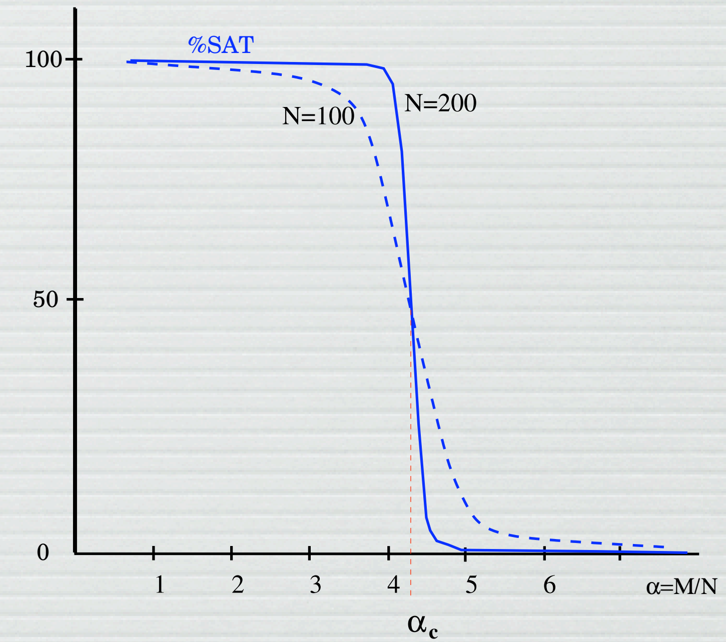
- BP: Best decoders for LDPC error correcting codes
- SP: Best solver of random Satisfiability problems
- BP: Best algorithm for learning patterns in neural networks (e.g. binary perceptron)
- Data clustering, graph coloring, Steiner trees, etc...



Local, simple update equations: Each message is updated using information from incoming messages on the same node. Distributed, solves hard global pb

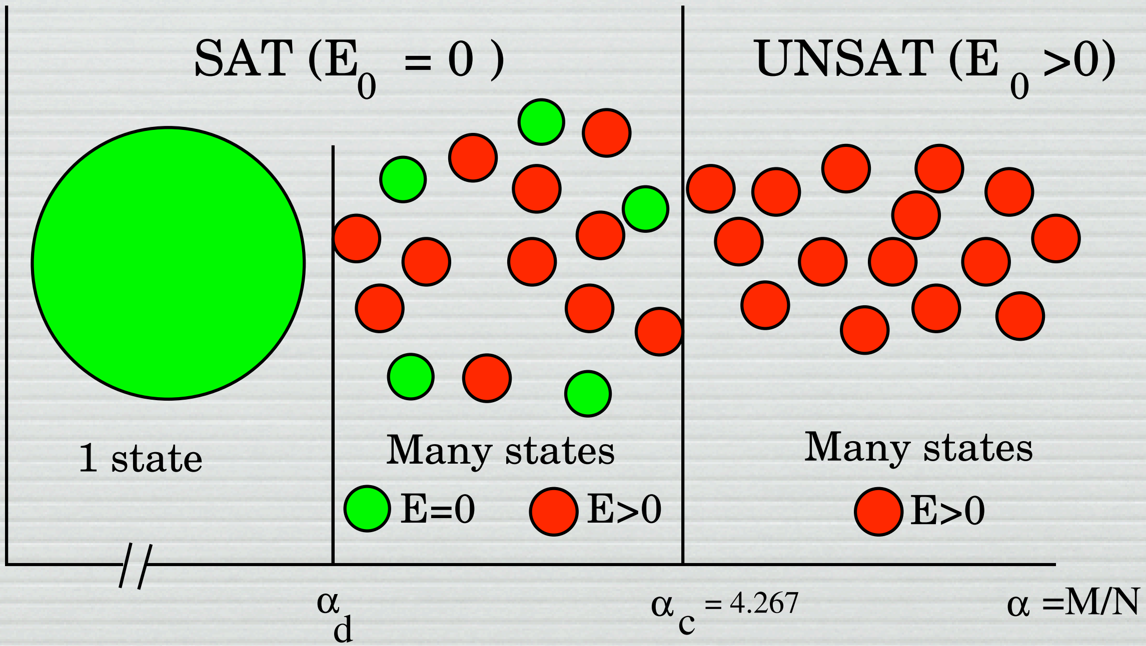
Random Satisfiability

SAT-UNSAT transition at the critical constraint density α_c



Intermediate clustered phase: $\alpha_D < \alpha < \alpha_c$

Many clusters of solutions, many more metastable states: only a-thermal algorithms



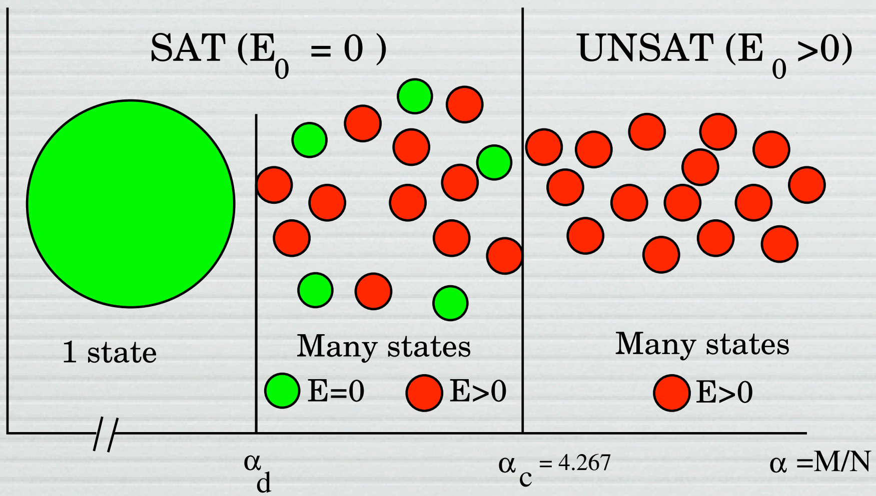
SP: solves instances of 10^7 close to α_c

Summary, Perspectives

- A broad class of problems related to information processing: many "simple" variables, local interactions
- Common framework: factor graph, message passing
- Common properties: phase transitions when the density of constraints/interactions increases
- Very powerful message passing algorithms
- Unexpected applications of spin glass theory, ubiquity of glass phases
- Appealing feature: simple local exchange of information. A "natural" class of a-thermal algorithms. Distributed computations, robust to noise (neural-like)

Summary, Perspectives

- Clustering of solution space close to the transition



Clustering also present in codes, in coloring, in learning from examples, ...

Cluster of solutions= working state of the system. Various working states, possibility to address clusters (data compression), to switch from one to another... Many perspectives, interface physics - computation

Collaborators

- A. Braunstein, S. Ciliberti, J. Chavas, S. Franz, C. Furtlehner, O. Martin, S. Mertens, A. Montanari, T. Mora, M. Mueller, M. Palassini, G. Parisi, F. Ricci-Tersenghi, O. Rivoire, M. Tarzia, C. Toninelli, M. Weigt, L. Zdeborova, R. Zecchina

References on my web page

http://www.lptms.u-psud.fr/membres/mezard/

+book at Oxford University Press:
"Information, Physics, and Computation"
by M. M. and A. Montanari