MECCANICA STATISTICA DEI PROBLEMI DI OTTIMIZZAZIONE COMBINATORIA

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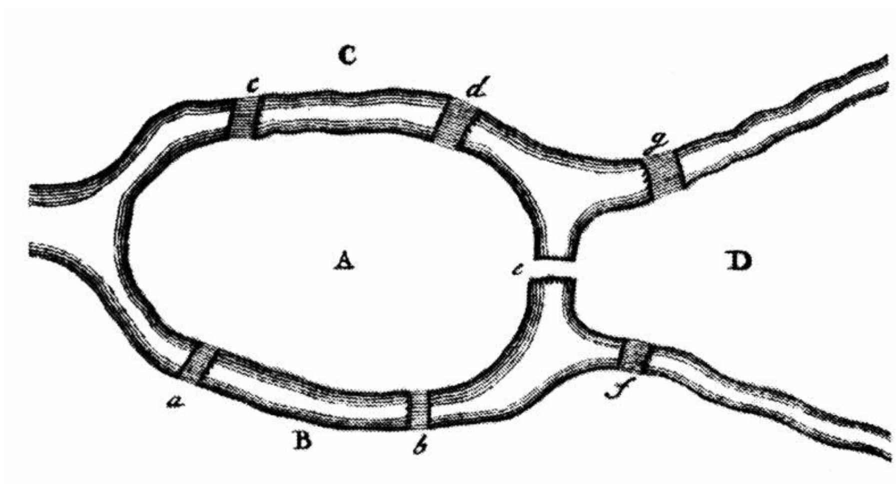
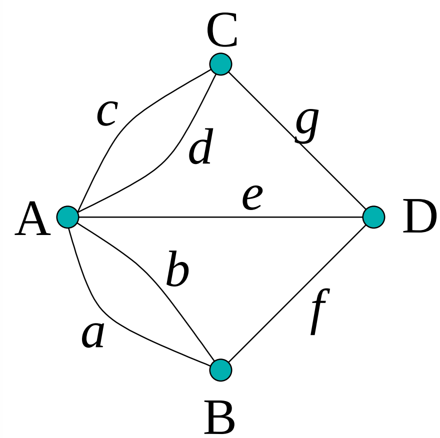
- Breve introduzione alla Complessità Computazionale
- Legame con la Meccanica Statistica
- Semplici nozioni sugli ipergrafi random
- Analisi di un modello semplice: 3-spin diluito
- Conclusioni, applicazioni e prospettive future

Two old decision problems

Eulerian circuits (1736)

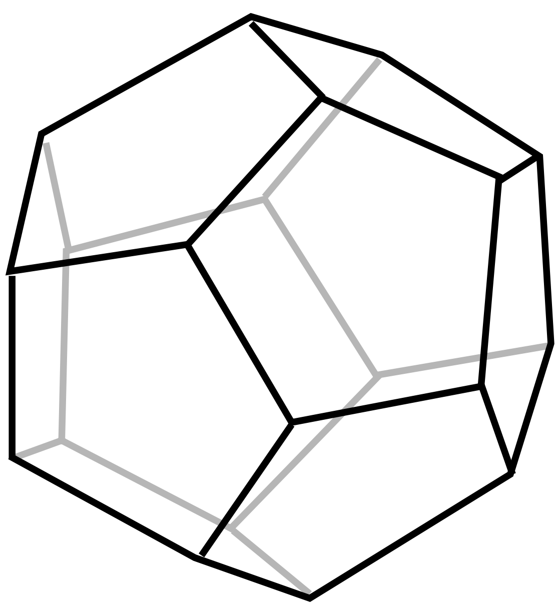


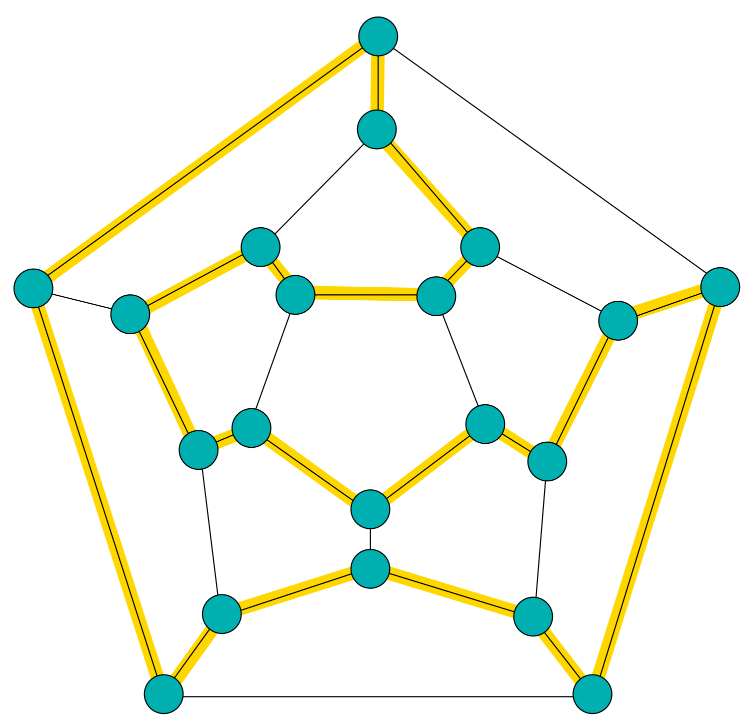


The seven bridges of Könisberg

The equivalent graph

Hamiltonian cycles (1859)





The dodecahedron

The equivalent graph

Computer Science: computational complexity

Classifying problems according to the computational resources required for their solution (e.g. CPU time and memory) in the worst case.

tractable (in P) $\leftrightarrow$ sub-exponential: $\ln(N)$, N^α
intractable (in NP) $\leftrightarrow$ exponential: 2^N, $N!$

N is the number of variables in the problem.

Main Complexity Classes

P = polynomial
NP = non-deterministic polynomial

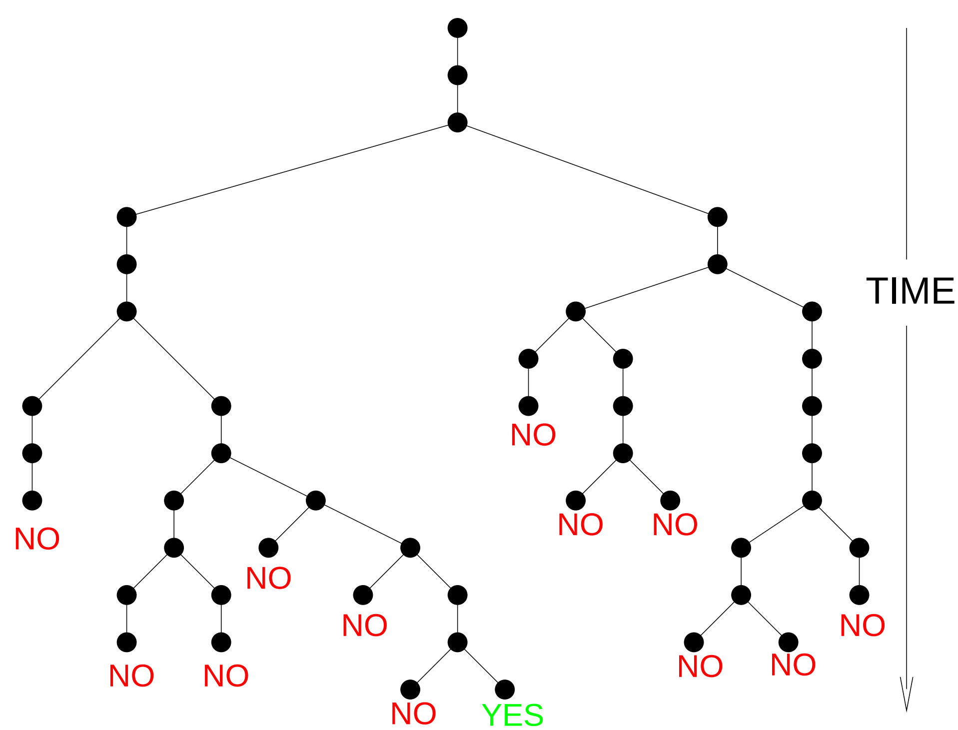
$\Downarrow$

- non-determ. algorithms: `goto both`
- succinct certificate

P = NP ?

First Millennium Prize Problem

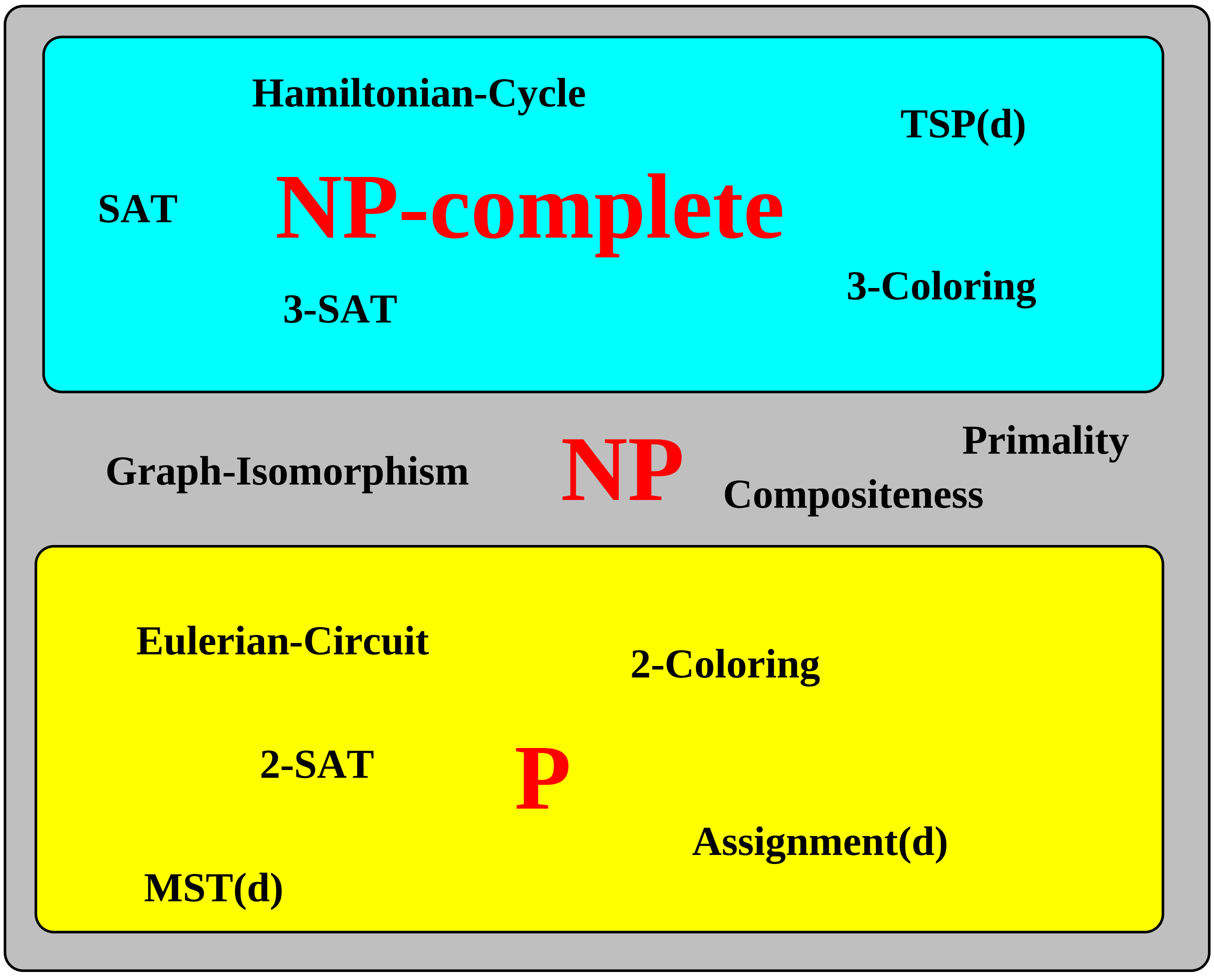
Quantum computation !



NP-completeness: combinatorial optimization

THEOREM: All problems in NP are polynomially reducible to K-SAT ($K > 2$). (Cook, 1971)

NP-complete are the hardest **NP** problems.



Beyond NP

- { decision, evaluation, optimization } problems (NP-hardness)
- counting problems (#P,#P-complete): e.g. #SAT counts the entropy of SAT.

Some interesting problems

SAT

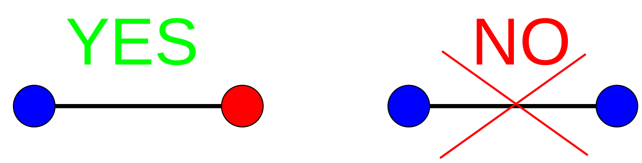
Boolean variables: $x_i \in \{0,1\} \quad i = 1, \ldots, N$
Logical operators: $\bar{\cdot}$ = NOT, $\vee$ = OR, $\wedge$ = AND
Given a Boolean formula like
$(x_1 \vee x_{27} \vee \bar{x}_3) \wedge (\bar{x}_{11} \vee x_2) \wedge \ldots \wedge (\bar{x}_{21} \vee x_9 \vee \bar{x}_8 \vee \bar{x}_{30})$
decide if a satisfying truth assignment exist

Random 3-SAT: 3 random literals per clause

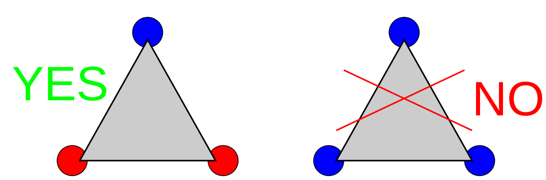
$$\# \text{ clauses} = \alpha N$$

Coloring

q-coloring on graphs:
2-coloring $\in$ P
3-coloring $\in$ NP-c



Bicoloring on hypergraphs:
NP-complete



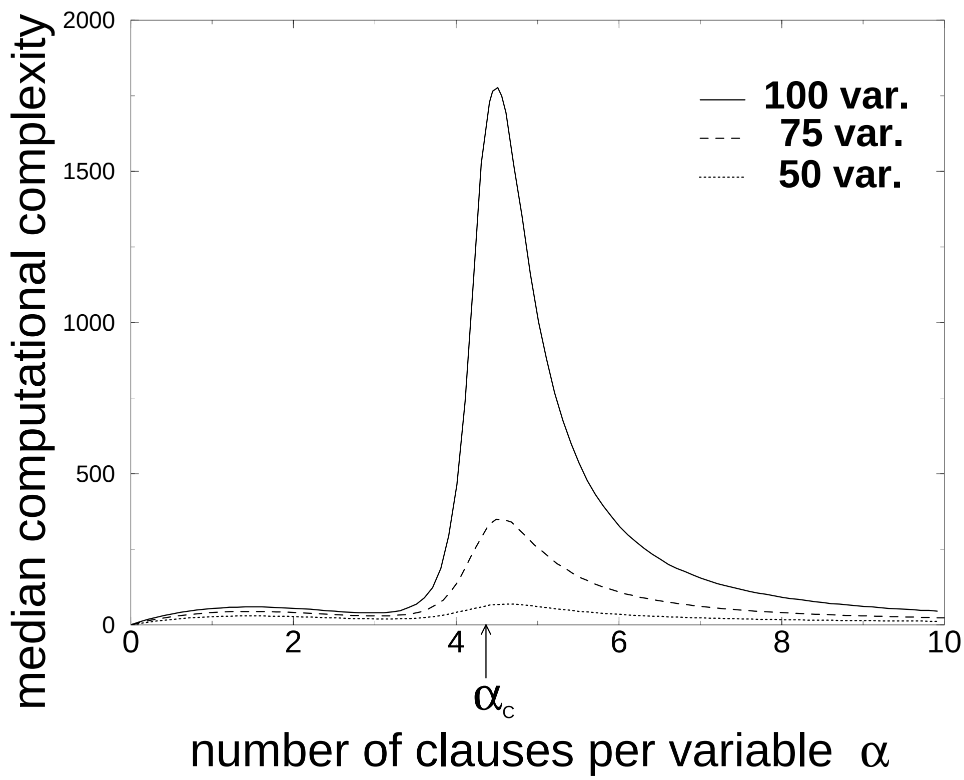
Computer Science	Physics
K-SAT	Diluted Ising Spin Glasses
Graph Coloring	Potts Models
Vertex Cover	Hard Spheres
...	...

Worst-case vs. Typical-case

Real-world NP-complete and #P-complete problems may have many easy instances

Ensemble of random NP-complete problems hard on average (e.g. random 3-SAT)

Random models: phase transitions, NP-hardness



Onset of complexity $\leftrightarrow$ Phase transition

SAT/UNSAT transition: $E = \#$ violated clauses becomes greater than zero.

What makes problems hard close to α_c?

Mapping to a Statistical Mechanics problem

Zero temperature limit of a diluted mean-field spin model. Much harder than usual fully connected!

For random 3-SAT, with $s_i = (-1)^{x_i}$,

$$\mathcal{H} = \frac{1}{8}\left(\alpha N - \sum_{i=1}^{N} H_i s_i + \sum_{i<j} T_{ij} s_i s_j - \sum_{i<j<k} J_{ijk} s_i s_j s_k\right)$$

$$\begin{aligned} H_i &= \textstyle\sum_\ell \Delta_{\ell,i} \\ T_{ij} &= \textstyle\sum_\ell \Delta_{\ell,i}\Delta_{\ell,j} \\ J_{ijk} &= \textstyle\sum_\ell \Delta_{\ell,i}\Delta_{\ell,j}\Delta_{\ell,k} \end{aligned} \qquad \Delta_{\ell,i} = \begin{cases} 1 & \text{if } \bar{x}_i \in C_\ell \\ -1 & \text{if } x_i \in C_\ell \\ 0 & \text{otherwise} \end{cases}$$

For 3-hyper-SAT also known as 3-XOR-SAT

$$F = (x_2 \oplus x_{15} \oplus x_{33}) \wedge \ldots \wedge (\bar{x}_4 \oplus \bar{x}_{21} \oplus \bar{x}_9)$$

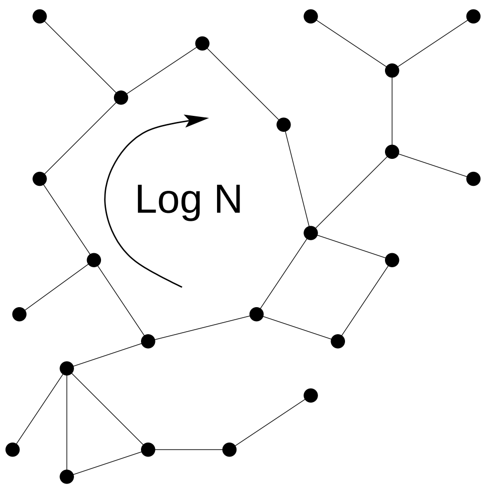
$$\mathcal{H} = \frac{1}{2}\left(\gamma N - \sum_{\{i,j,k\}\in G} J_{ijk}\, s_i\, s_j\, s_k\right)$$

$G = \{\text{set of } \gamma N \text{ random triples}\}$

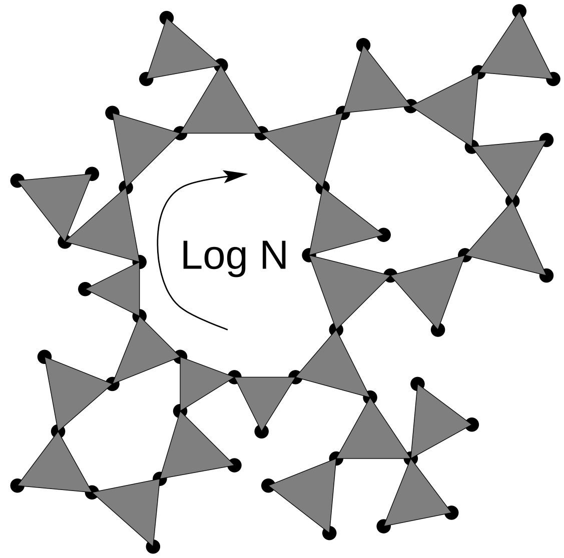
Two versions:

- unfrustrated, ferromagnetic: $J_{ijk} = 1$
  $\rightarrow$ 1st order ferromagnetic transition
- frustrated, 3-spin glass: $J_{ijk} = \pm 1$
  $\rightarrow$ SAT/UNSAT transition

Graphs and Hypergraphs



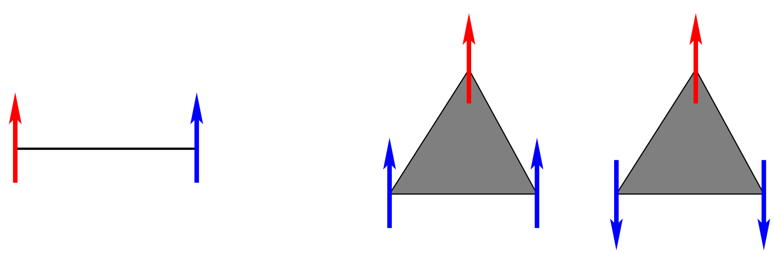
Graph (2−spin interactions)



Hypergraph (3−spin interactions)

Typically they are non planar and long range:
typical loops are of order $\ln(N)$

How to satisfy
a ferromagnetic
interaction

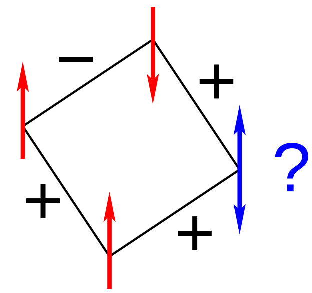


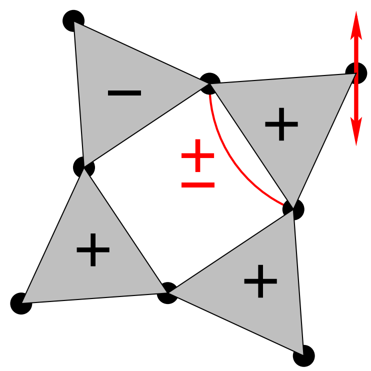
Finding the ground state of an unfrustrated spin model is an easy problem on a graph, but it may be hard on a hypergraph

Very different $T = 0$ dynamics (coarsening)

Frustration $\leftrightarrow$ $J = \pm 1$

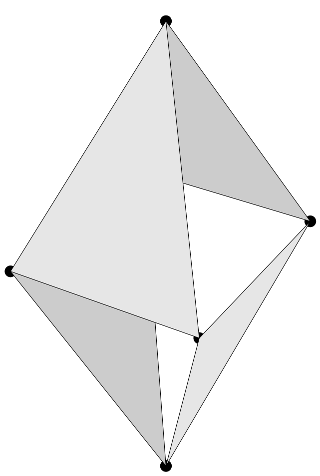
On a graph the frustration arises with loops at the percolation point ($\gamma_p = 1/2$). On a hypergraph the loops arising a the percolation point ($\gamma_p = 1/6$) give no frustration.





Spin on dangling ends can be freely fixed in order to change the effective interaction between the other two spins. Only **hyperloops** can generate frustration on a hypergraph.

Definition of hyperloop: a non-empty set $\mathcal{S}$ of hyperlinks $\{i, j, k\}$ such that every node (spin) appears in $\mathcal{S}$ an even number of times (zero is even).

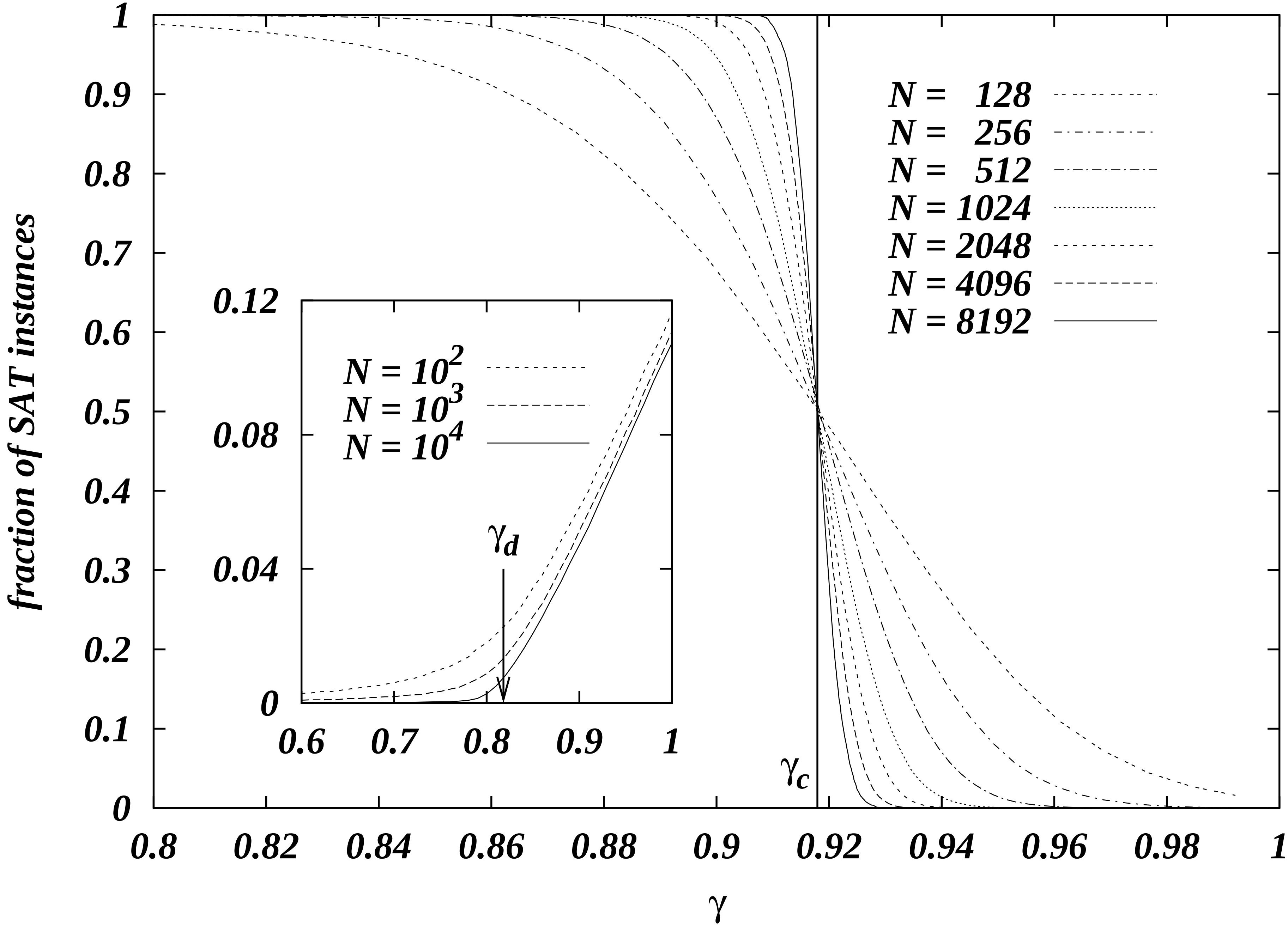


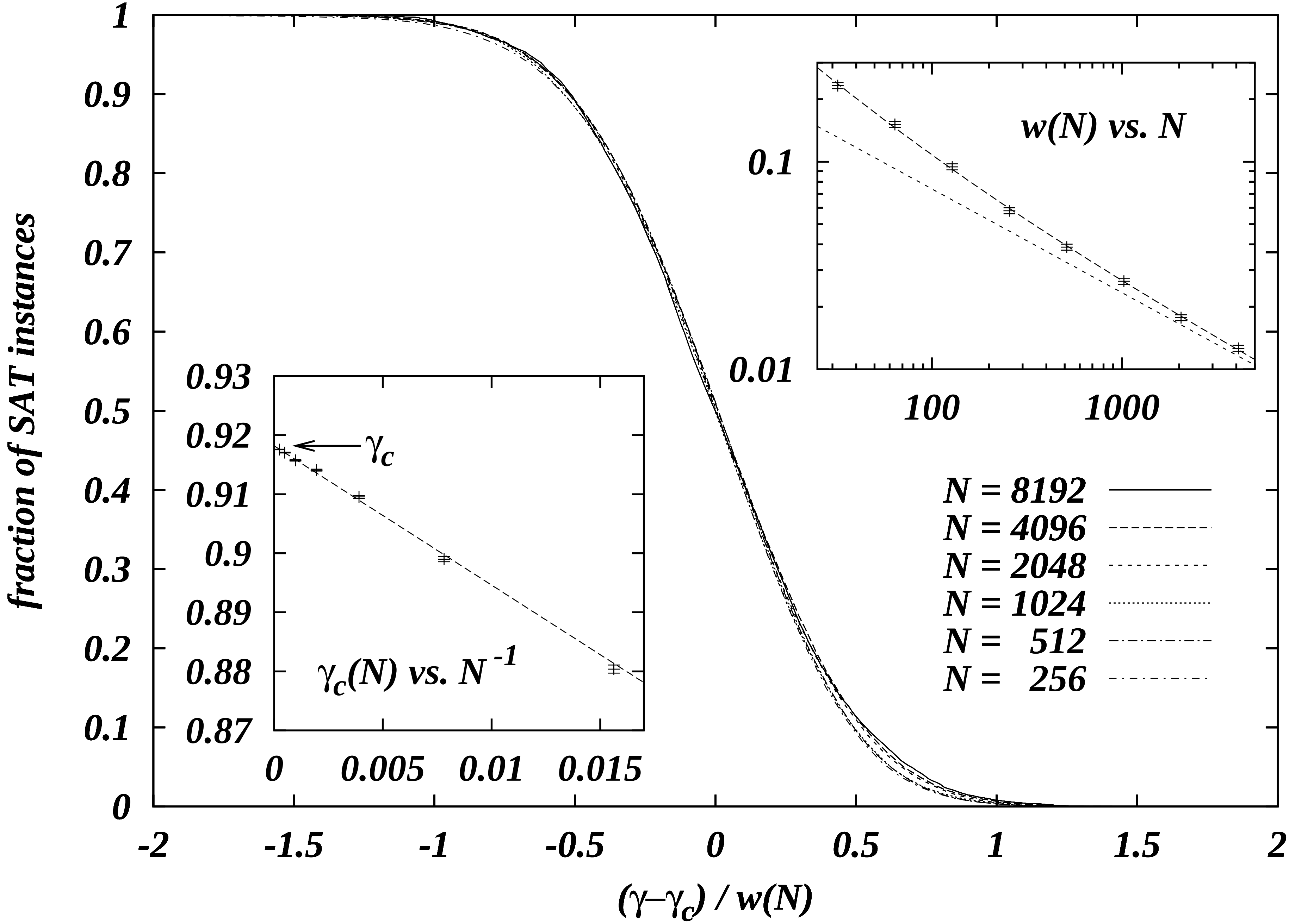
hyperloops $\Rightarrow$ frustration

satisfied interaction: $J_{ijk} s_i s_j s_k = 1$

$$1 = \prod_{\{i,j,k\} \in \mathcal{S}} J_{ijk}\, s_i\, s_j\, s_k =$$

$$= \prod_{\{i,j,k\} \in \mathcal{S}} J_{ijk} = \begin{cases} 1 & p = 1/2 \\ -1 & p = 1/2 \end{cases}$$


fraction of SAT instances
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.8
0.82
0.84
0.86
0.88
0.9
0.92
0.94
0.96
0.98
1
γ
γ_c
N = 128
N = 256
N = 512
N = 1024
N = 2048
N = 4096
N = 8192
0.12
0.08
0.04
0
0.6
0.7
0.8
0.9
1
$N = 10^2$
$N = 10^3$
$N = 10^4$
γ_d


fraction of SAT instances
(γ−γc) / w(N)
w(N) vs. N
γc(N) vs. N -1
γc
N = 8192
N = 4096
N = 2048
N = 1024
N = 512
N = 256

Unfrustrated model: $J = 1$

The existence of a ferromagnetic solution follows from a simple argument

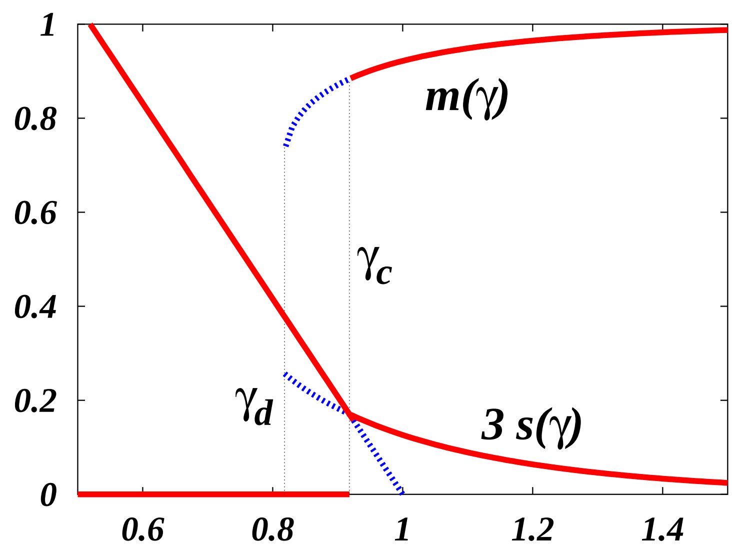
$$1 - m = \sum_c e^{-3\gamma} \frac{(3\gamma)^c}{c!} \frac{c}{3\gamma} (1 - m^2)^{c-1} = e^{-3\gamma m^2}$$

Up to $\gamma_d = 0.818$ the hypergraph is like a tree

$m(\gamma)$ is the fraction of frozen spins, i.e. the magnetization

$s(\gamma)$ is the entropy

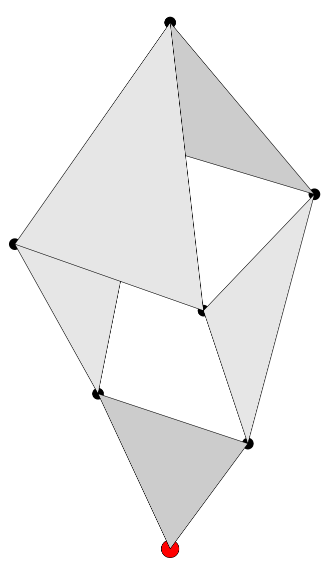
$\gamma_c = 0.918$



The difficult task is to calculate $s(\gamma) \to$ replicas!

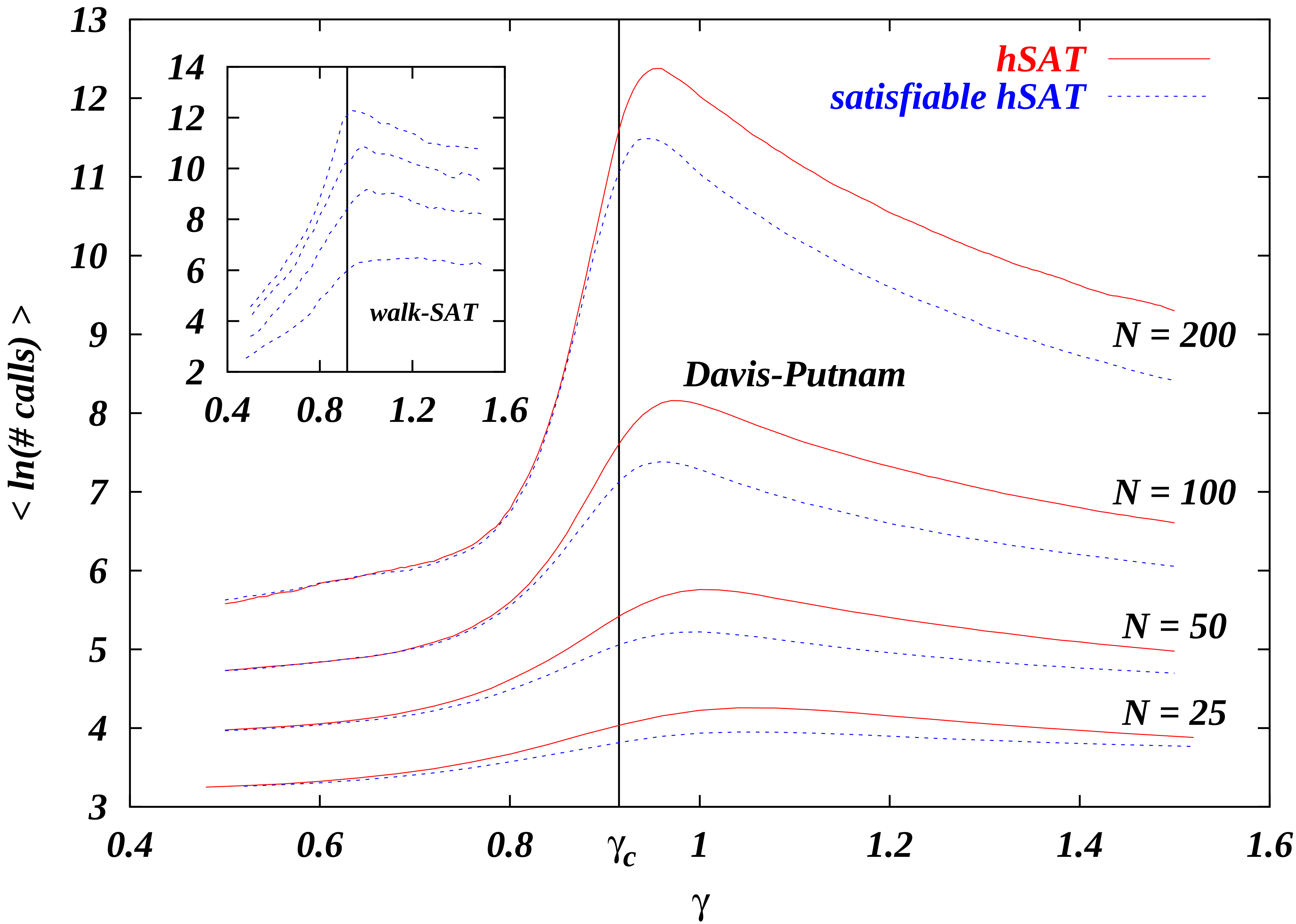
$$s(\gamma) = \ln(2)[1 - \gamma - m + 3\gamma m^2 (1 - m) + \gamma m^3]$$

Challenge for mathematicians: calculate γ_c without replicas



At γ_c percolate hyperloops and **hyperfields $\Rightarrow$ magnetization**

$$s_\ell = \prod_{\{i,j,k\} \in \mathcal{T}} s_i\, s_j\, s_k = \prod_{\{i,j,k\} \in \mathcal{T}} J_{ijk} = 1$$


hSAT
satisfiable hSAT
Davis-Putnam
N = 200
N = 100
N = 50
N = 25
walk-SAT
< ln(# calls) >
γ
γc
0.4
0.6
0.8
1
1.2
1.4
1.6
3
4
5
6
7
8
9
10
11
12
13
2
14

The structure of the configurational space

$x_i, \eta_{ijk} \in \{0,1\}$ $s_i = (-1)^{x_i}$ $J_{ijk} = (-1)^{\eta_{ijk}}$

$\{s_i\}$ is a solution $\Longleftrightarrow \forall \{i,j,k\} \in I \quad s_i s_j s_k = J_{ijk} \Leftrightarrow$

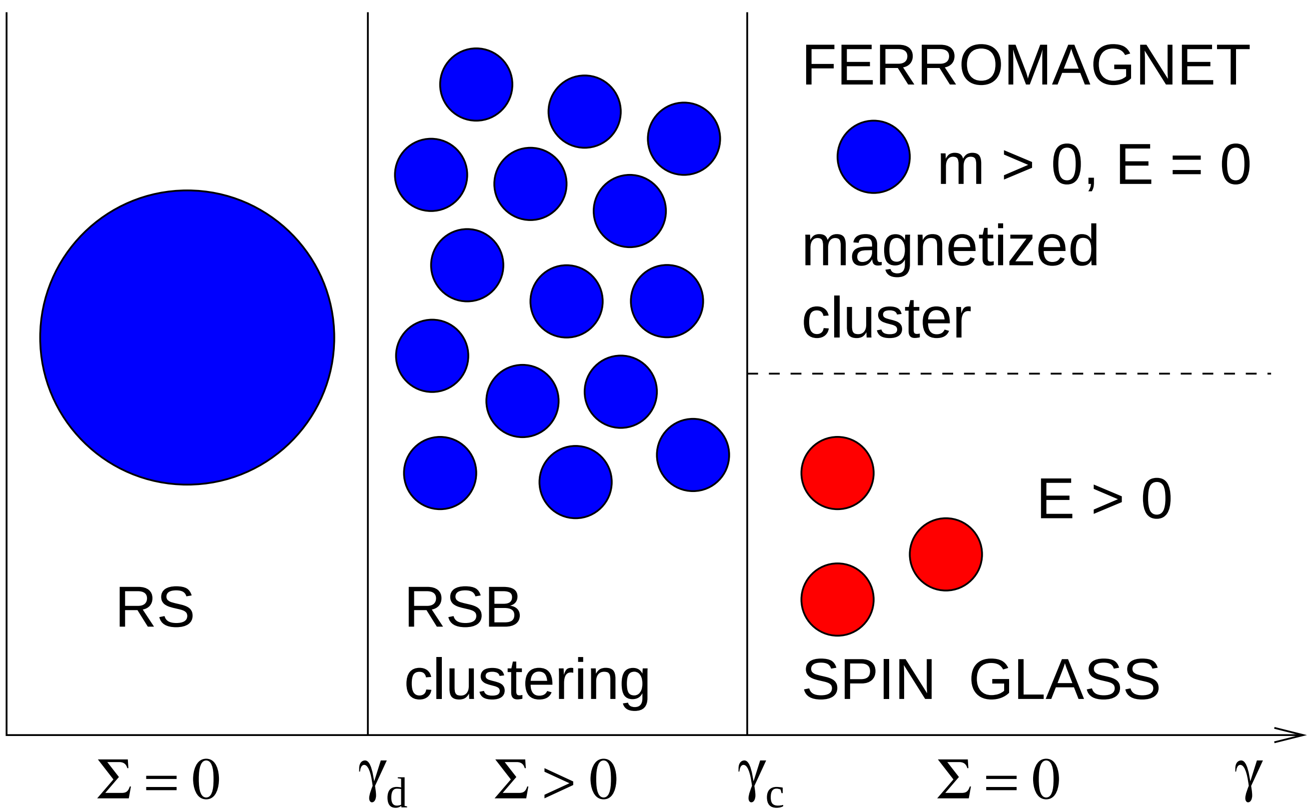
$\Longleftrightarrow (x_i \oplus x_j \oplus x_k) = \boxed{x_i + x_j + x_k (\text{mod } 2) = \eta_{ijk}}$

A common problem: diluted p-spin glass ≡ random p-XOR-SAT* (or low density Parity Check codes) ≡ random linear systems in finite fields (GF[2])

*considered an open problem in theoretical computer science

If $E = 0$ (no frustration) → Gaussian elimination

If $E > 0$ → exhaustive enumerations

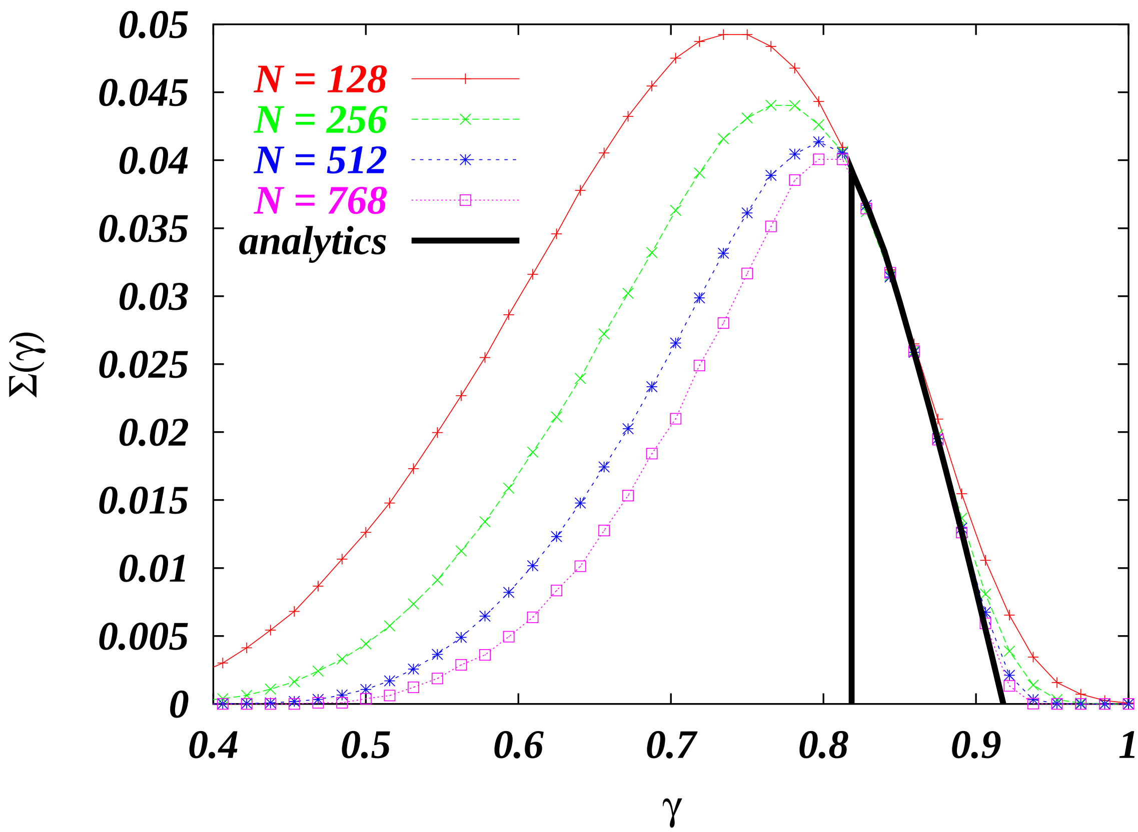


Configurational entropy: $\Sigma(\gamma) = \frac{1}{N} \ln(\#\text{ clusters})$

Configurational entropy: $\Sigma(\gamma) = \frac{1}{N} \ln(\# \text{ clusters})$
Since all clusters are equal

$$\begin{aligned}\Sigma(\gamma) &= \ln(2)(1-\gamma) - s(\gamma) = \\ &= \ln(2)\left[r - 3\gamma r^2(1-r) - \gamma r^3\right]\end{aligned}$$

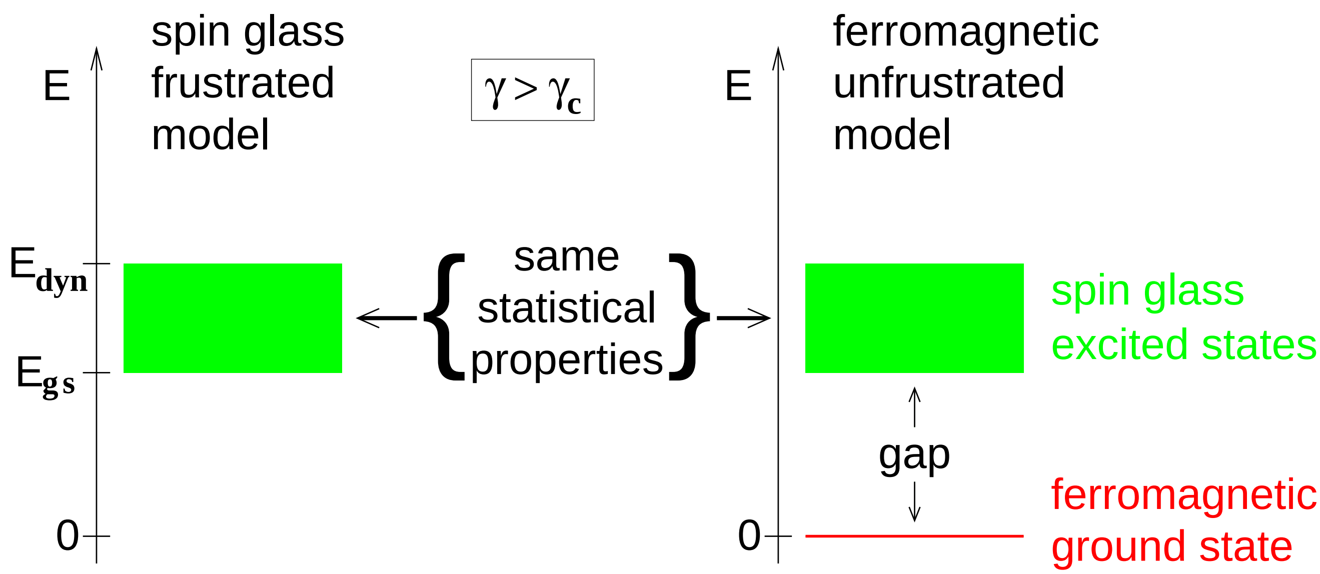
with $1 - r = \exp(-3\gamma r^2)$, is exact !



$\Sigma(\gamma) > 0$ for $\gamma \in [\gamma_d, \gamma_c]$ $\Rightarrow$

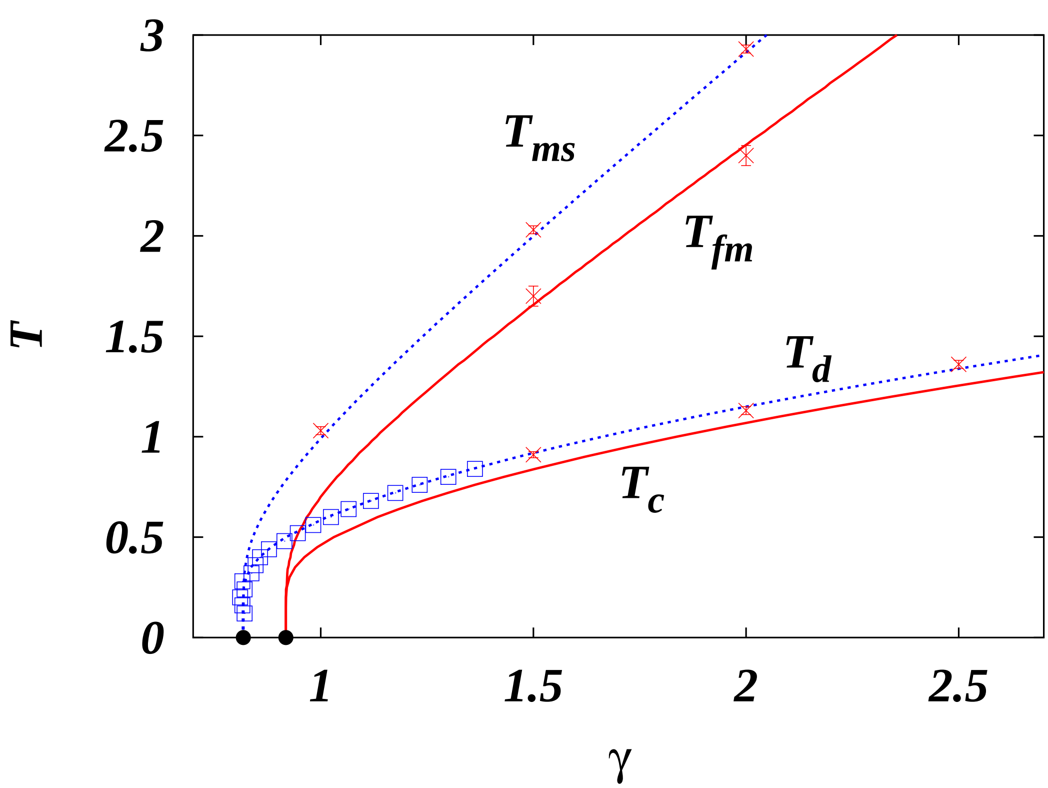
$\Rightarrow$ clustering and search algorithms slowing down
$\Rightarrow$ γ_c = SAT/UNSAT threshold for 3-XOR-SAT
$\Rightarrow$ dynamical transition in memory requirements [$\mathcal{O}(N) \to \mathcal{O}(N^2)$] solving linear systems in GF[2]

The structure of the configurational space

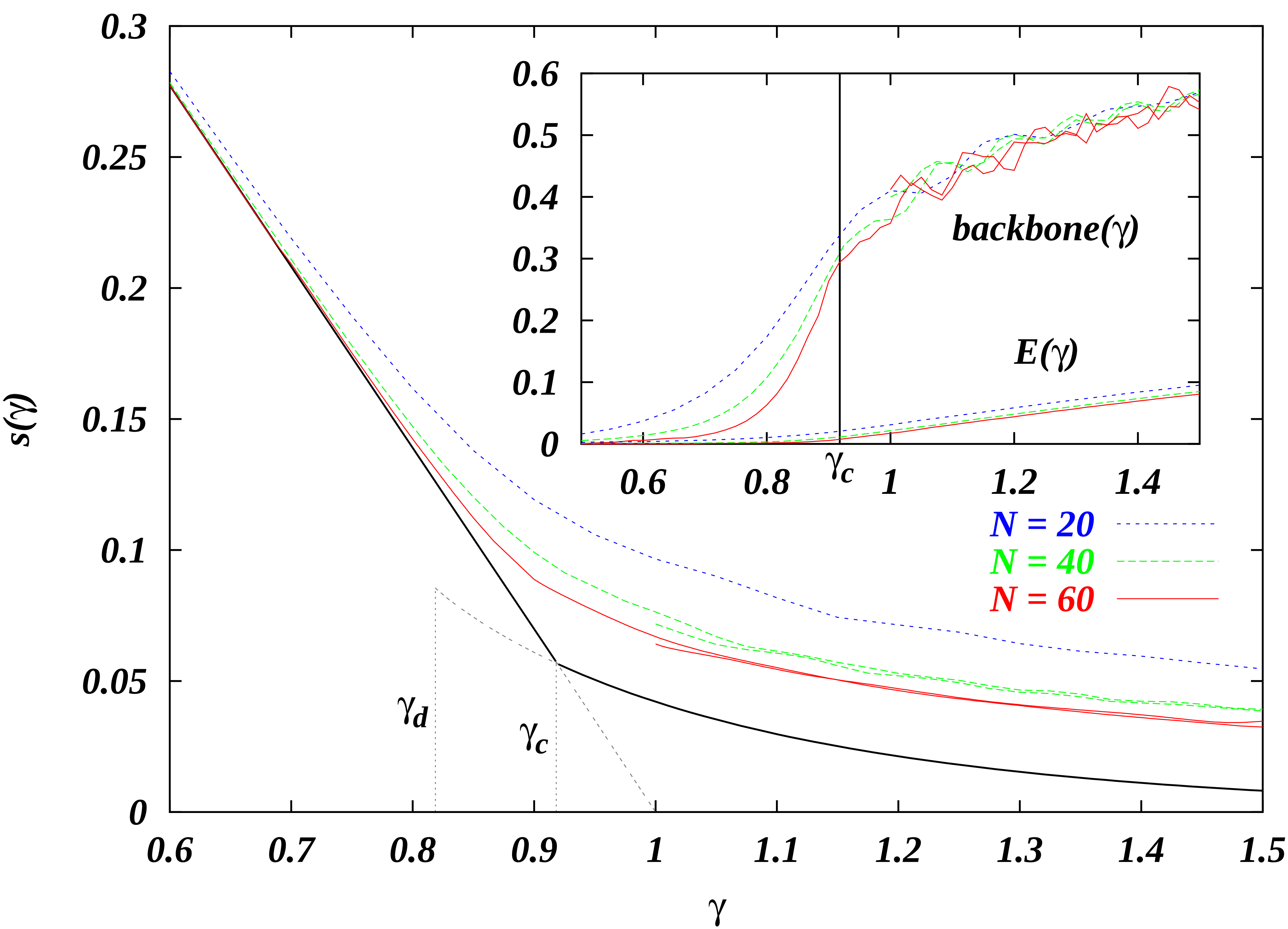


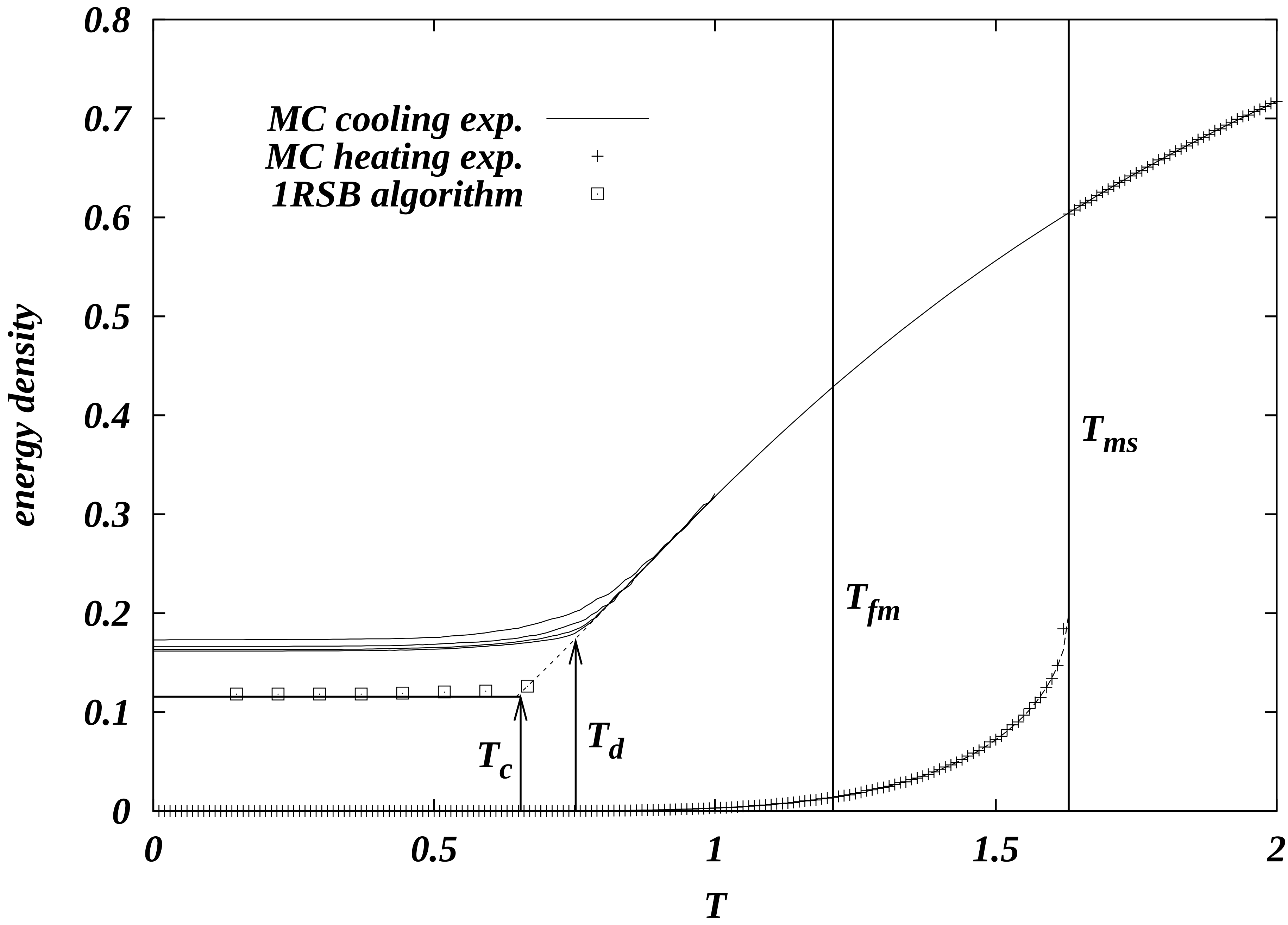
Starting from a random configuration, both models have the same off-equilibrium dynamics

Phase diagram



T is the temperature and 3γ is the average connectivity


s(γ)
γ
γd
γc
backbone(γ)
E(γ)
N = 20
N = 40
N = 60
0.3
0.25
0.2
0.15
0.1
0.05
0
0.6
0.7
0.8
0.9
1
1.1
1.2
1.3
1.4
1.5
0.6
0.5
0.4
0.3
0.2
0.1
0
0.6
0.8
1
1.2
1.4


MC cooling exp.
MC heating exp.
1RSB algorithm
energy density
T
T_c
T_d
T_{fm}
T_{ms}
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0
0.5
1
1.5
2

Conclusions and perspectives

New results

- p-spin ($p > 2$) with fluctuating connectivity

→ structure of the configurational space: γ_d, γ_c and $\Sigma(\gamma)$

→ γ_c is the exact threshold for random p-XOR-SAT

→ new transitions in random hypergraphs

- p-spin ($p > 2$) and Bicoloring with fixed connectivity

→ exact 1-RSB solution: GS energy

- K-SAT and Bicoloring

→ variational bounds for α_c (at present the best!)

Some applications

- test-bed for heuristic algorithms: GS energy
- dynamical transitions in Coding and Cryptography
- solvable models for glassy systems and granular matter

Examples of open issues

- complete 1-RSB and FRSB theories (with correlations)
- out of equilibrium dynamics
- analysis of randomized algorithms
- better analysis of the configurational space in K-SAT

Some references

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