自旋玻璃体系模拟

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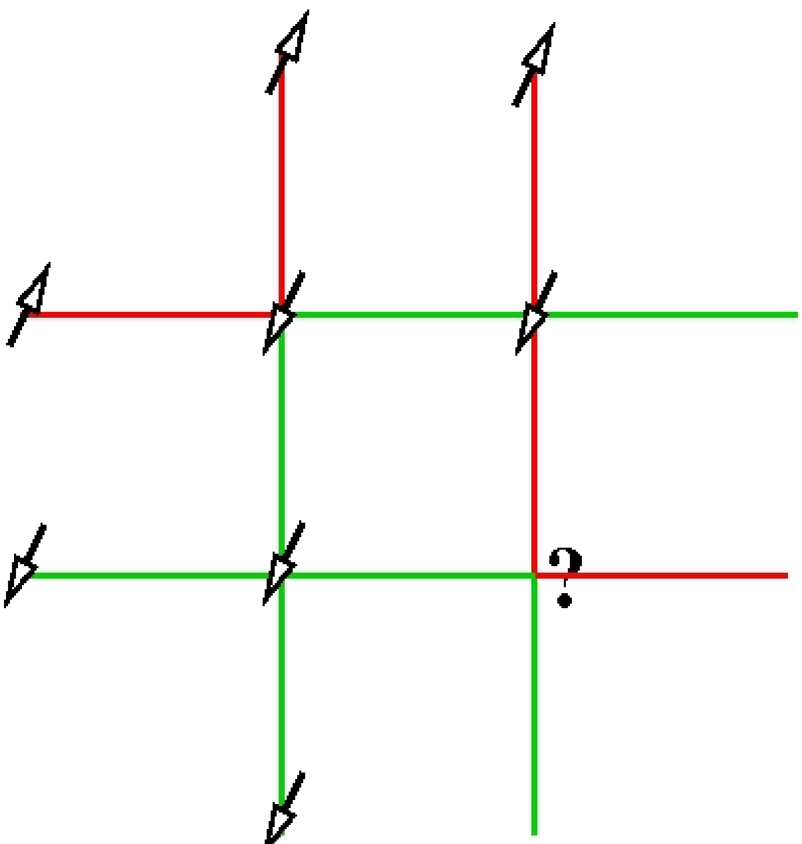
何谓自旋玻璃

$$H = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j$$



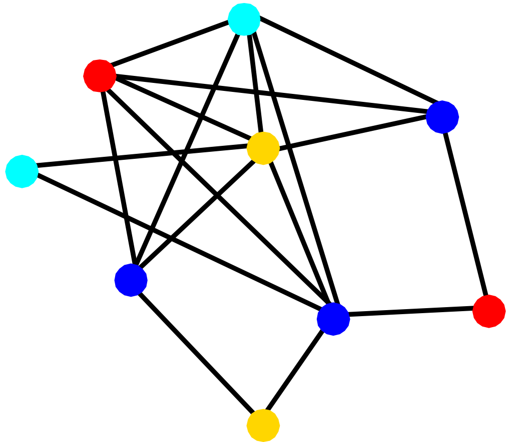
- 无序系统的简单模型

- 无序
- 竞争导致阻错

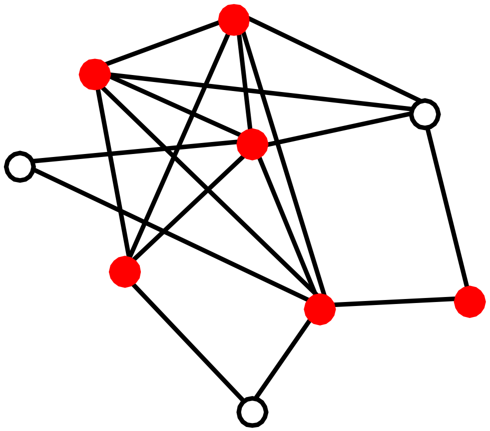
- 两体相互作用或多体相互作用

计算机科学中的对应问题：组合优化与约束满足

Q-COLoring

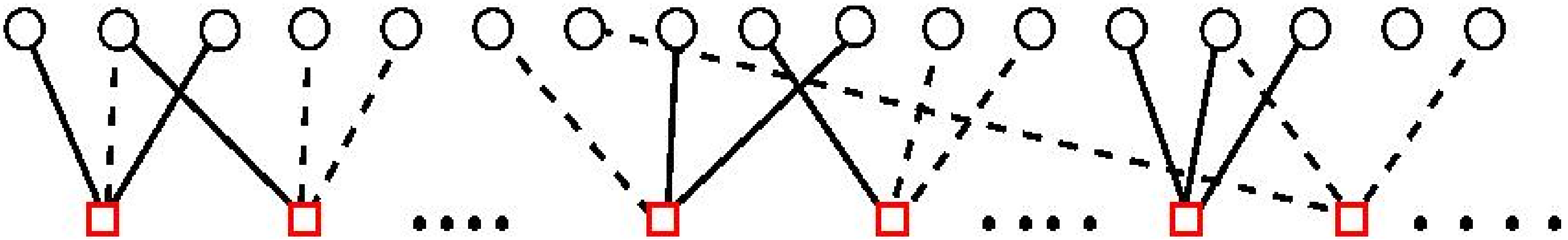


Vertex **C**over



Both are NP-complete problems,
NP-complete problems can be very difficult

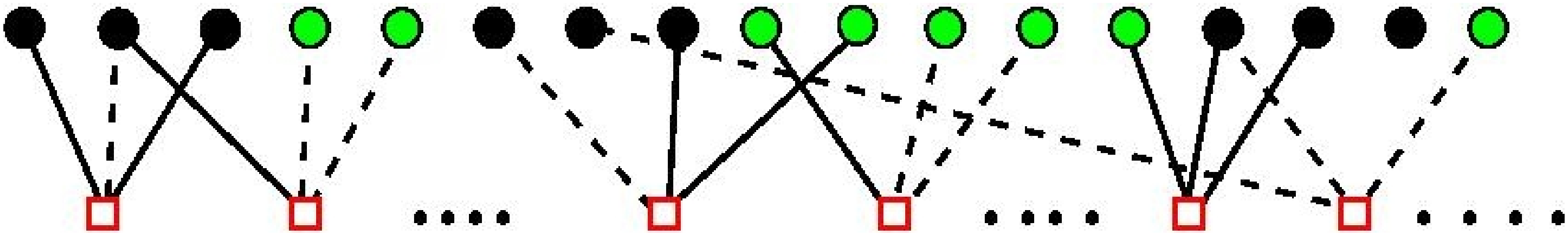
K-SAT



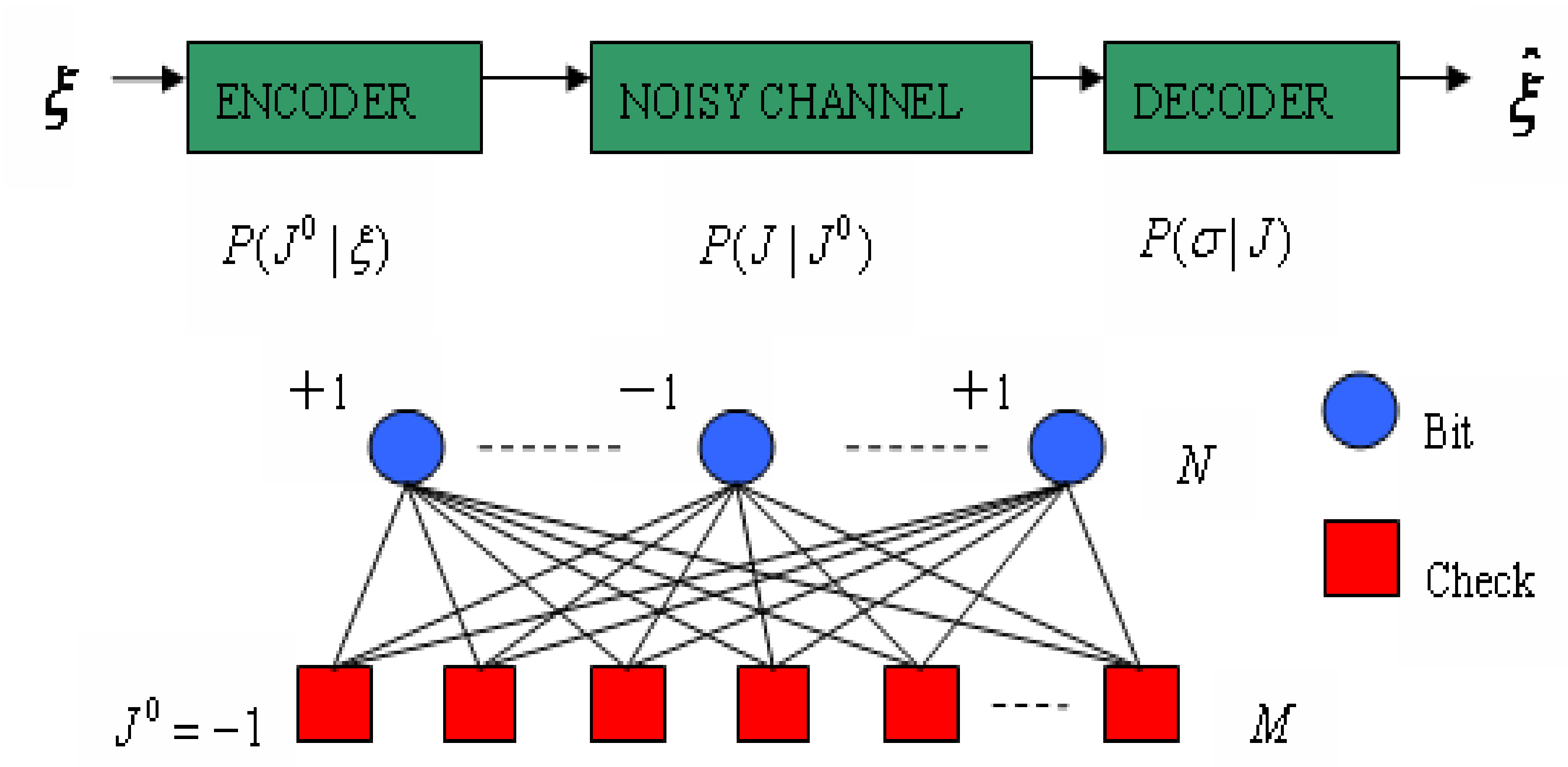
N binary variables:
M clauses:

constraint density α=M/N

a sat solution: black (true), green (false)



编码和解码：Low-density-parity-check codes



自旋玻璃体系构象空间的相变

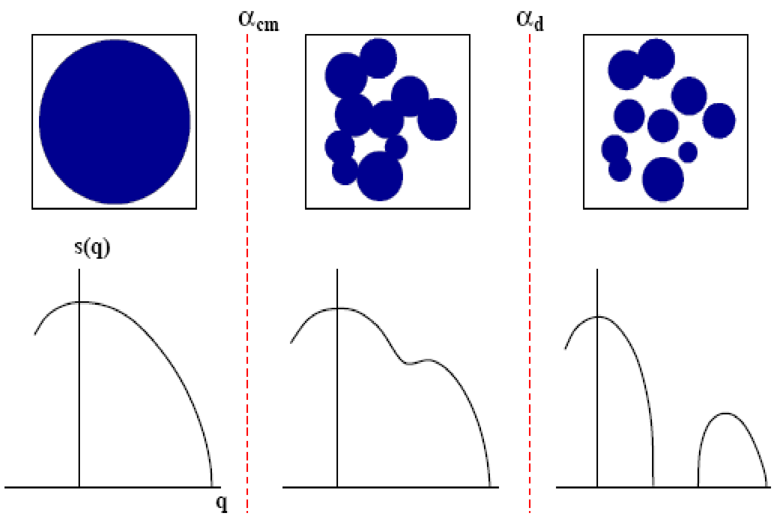


FIG. 1: (Color online) Evolution of the solution space $\mathcal{S}$ of a constrained spin system: At low constraint density α (left panel), $\mathcal{S}$ is homogeneous and the solution-pair entropy density $s(q)$ is a concave function of the overlap q. Solution communities start to form as α exceeds a threshold value α_{cm} (middle panel); $\mathcal{S}$ then becomes heterogeneous and the function $s(q)$ changes to be non-concave. An ergodicity-breaking transition occurs as α reaches a larger threshold value α_d (right panel), where the solution communities separate into different solution clusters and there are no solution-pairs with intermediate overlap values.

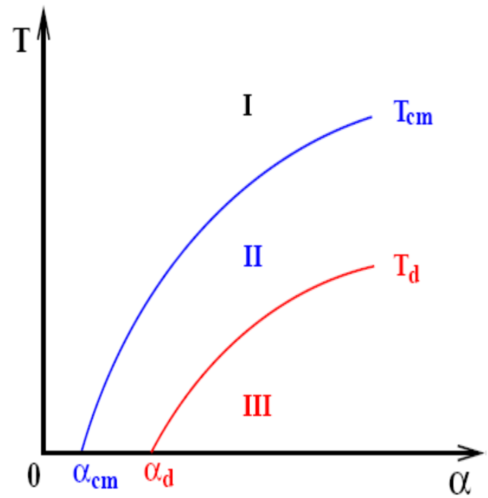
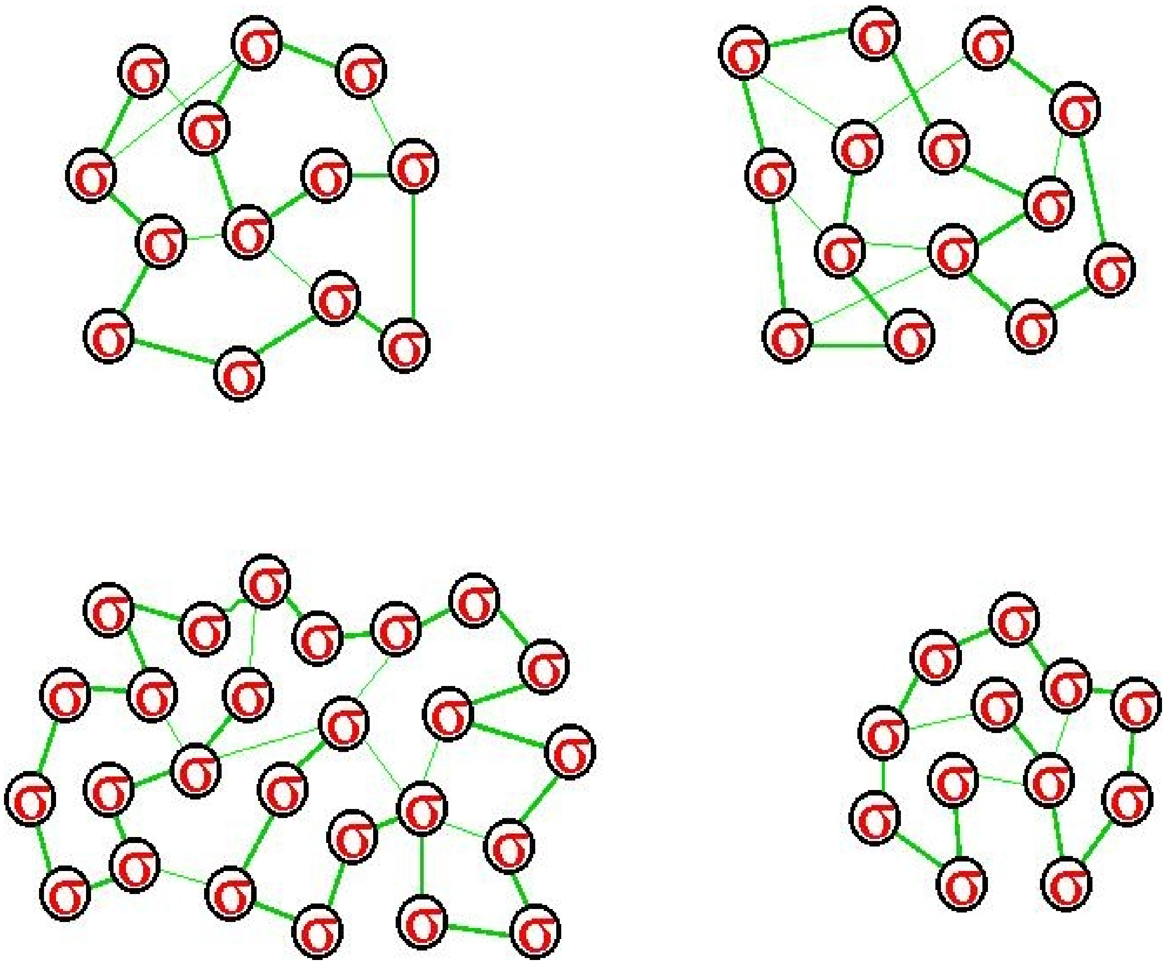


Fig. 4. Schematic phase diagram for a constraint satisfaction problem, using temperature T and constraint density α as control parameters. The configuration space is homogeneous and ergodic in region I. As the temperature T decreases to $T_{cm}(\alpha)$, a homogeneity-breaking transition occurs, and the configuration space becomes non-homogeneous but still ergodic (region II). As T further decreases to $T_d(\alpha)$, an ergodicity-breaking (clustering) transition occurs, and the configuration space breaks into many separated clusters (region III). At $T = 0$, the ground-state configuration space is non-homogeneous at $\alpha \geq \alpha_{cm}$ and non-ergodic at $\alpha \geq \alpha_d$.

understanding
solution/configuration space complex structures



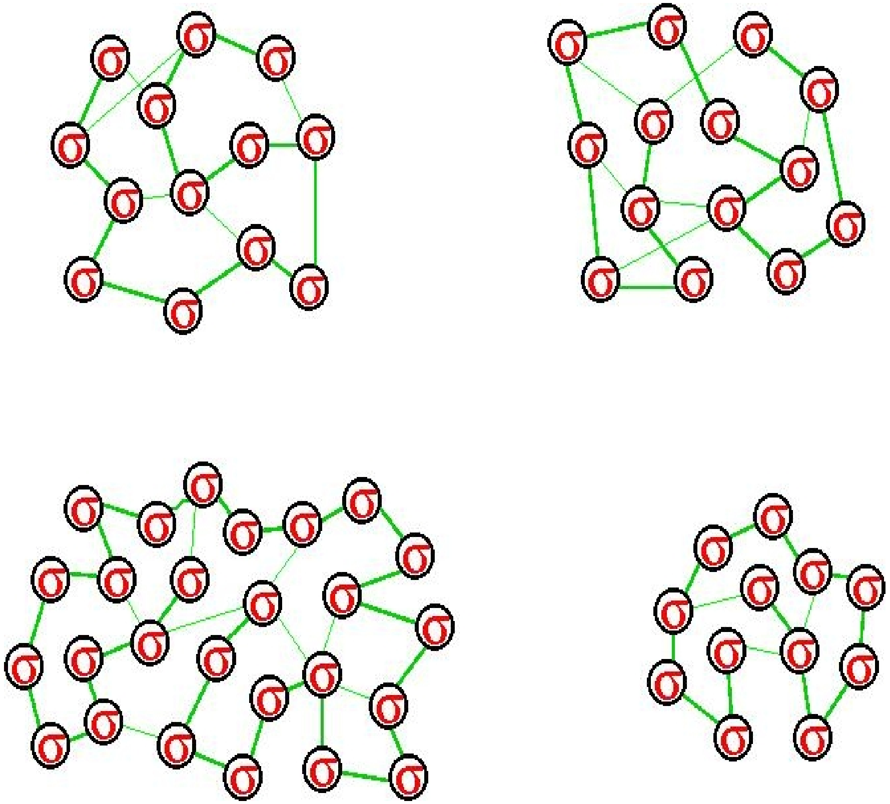
solution is N-dimension

σ={0/1,0/1,.....,0/1}

two solutions are connected by an edge if their Hamming distance is unity

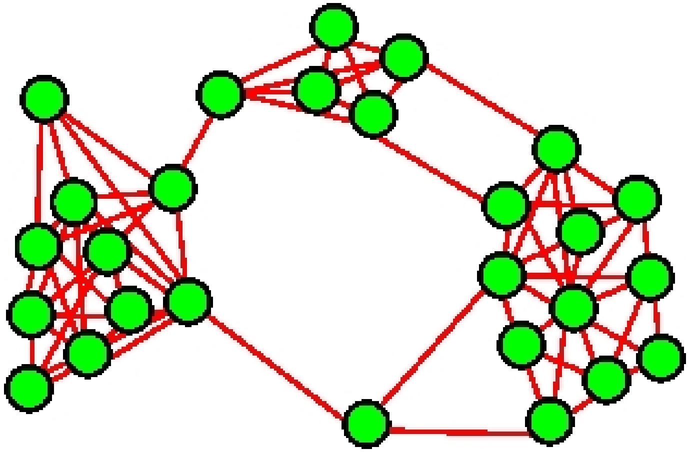
solution clusters!

Our questions



I.-- Fine structure in a single solution cluster (community structures)

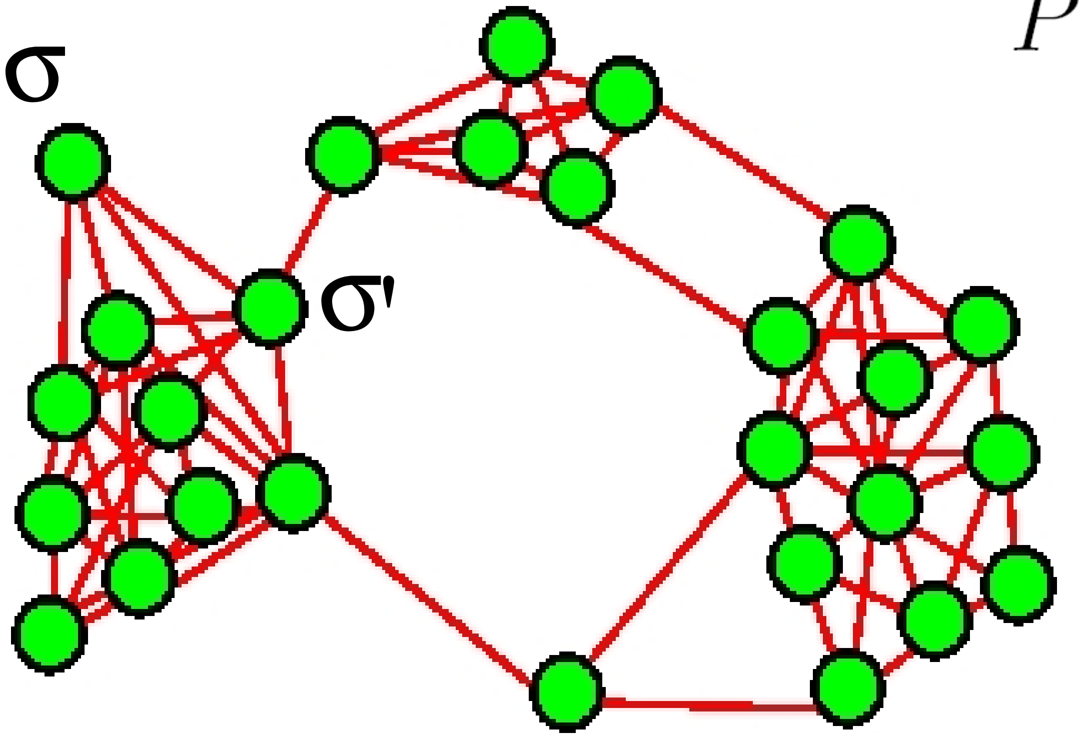
II.-- The influence of solution cluster fine structure to a stochastic search algorithm (SEQSAT)



How to detect the structure of a single cluster?

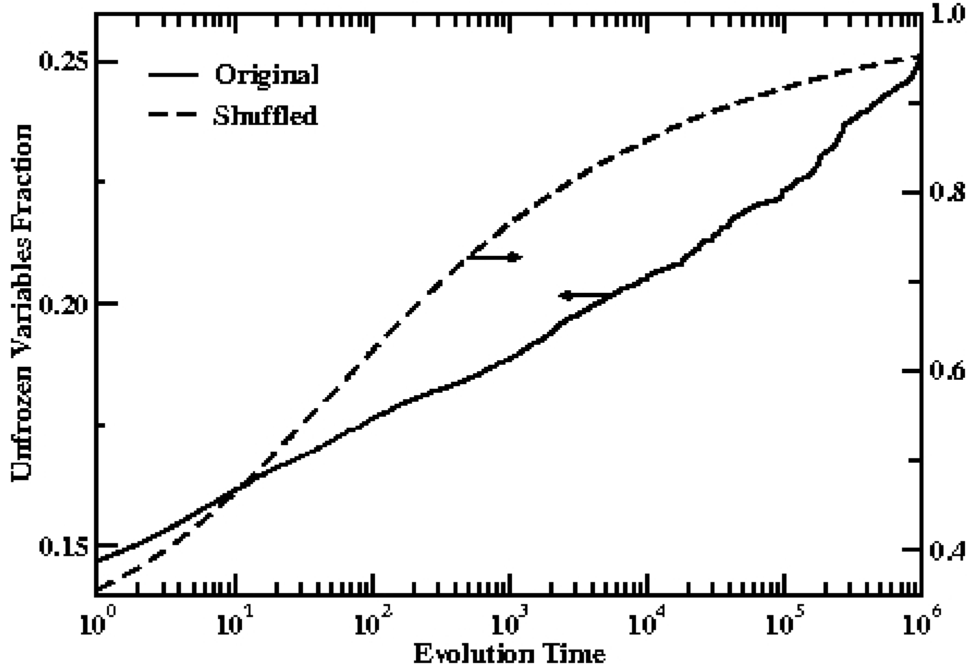
Enumeration is hopeless, as the graph is too large!

Our approach: solution cluster random walking



$$P(\sigma \to \sigma') = \frac{1}{|\partial \sigma|}$$

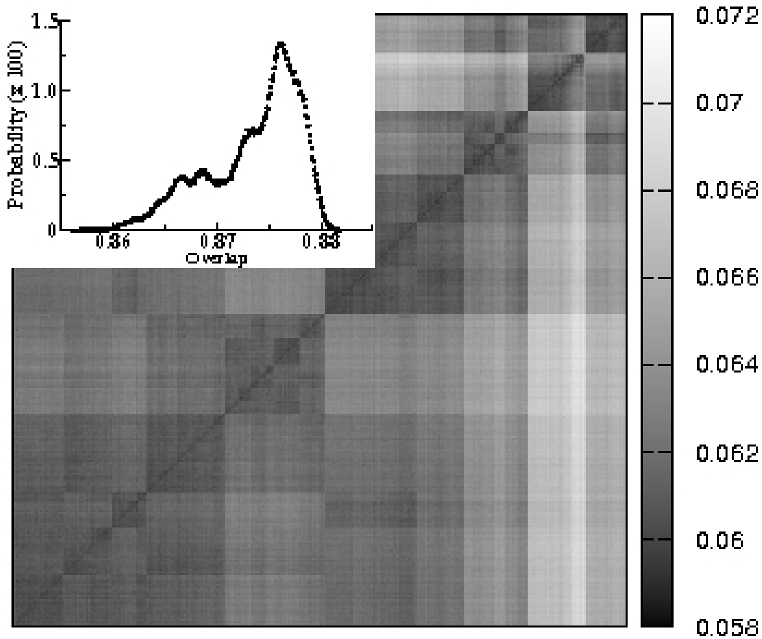
A

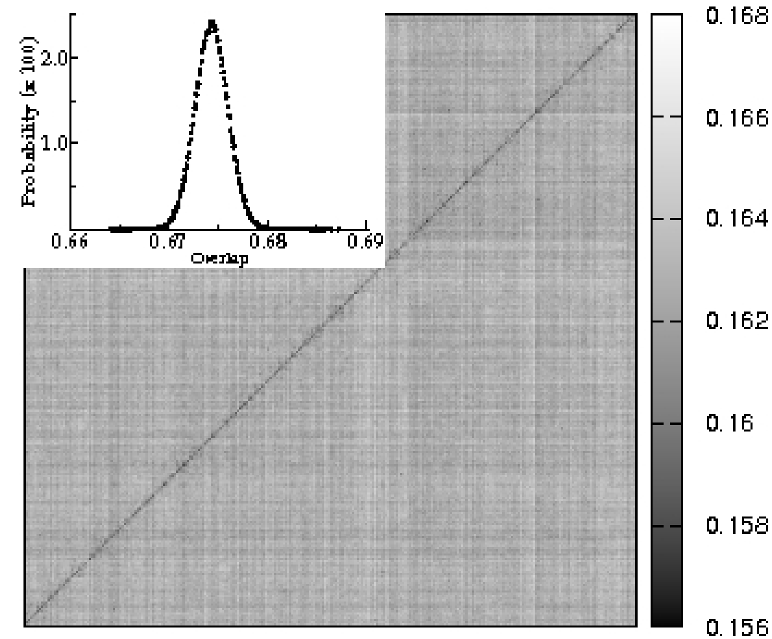


K=3
N= 1,000,000
M=4,200,000
alpha=4.25

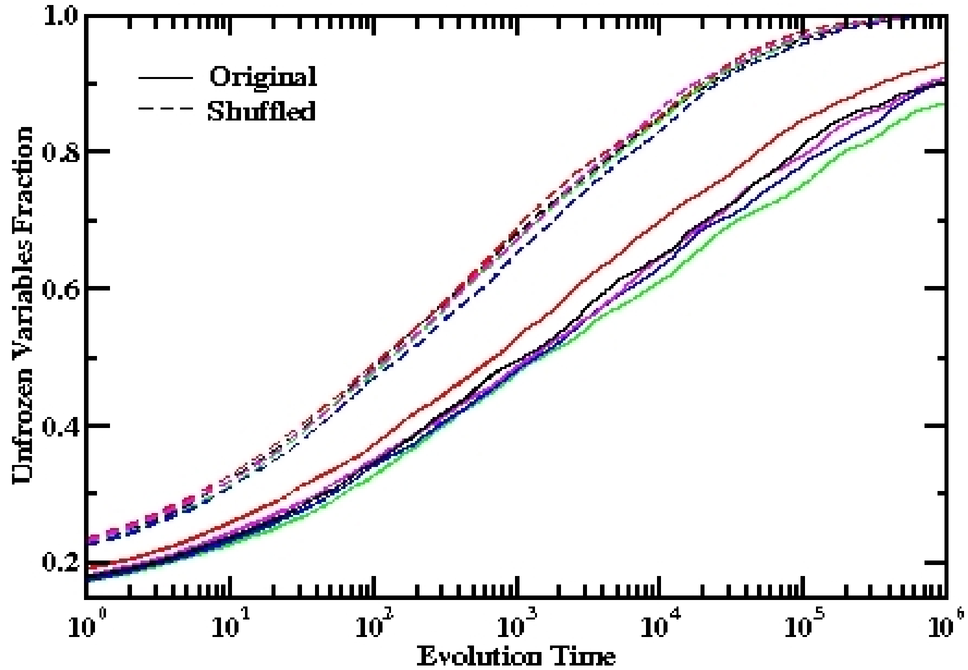
Original formula

A specially randomized version



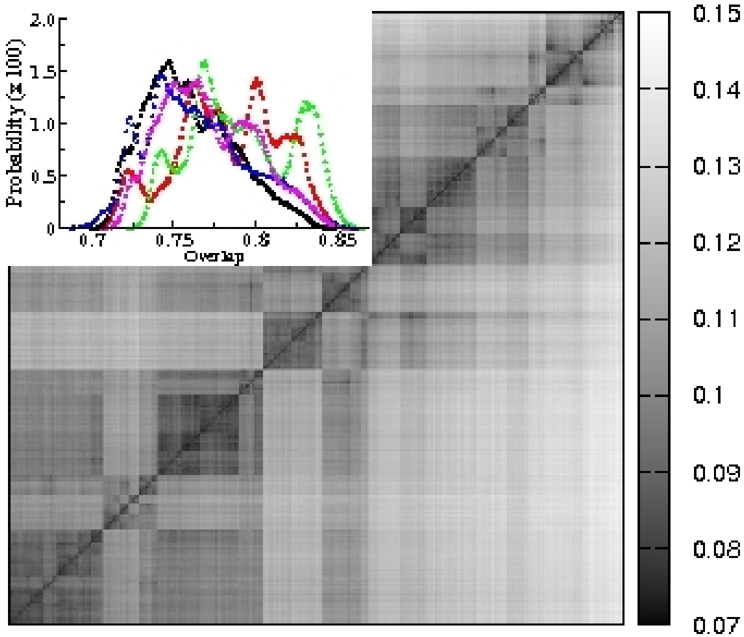


B

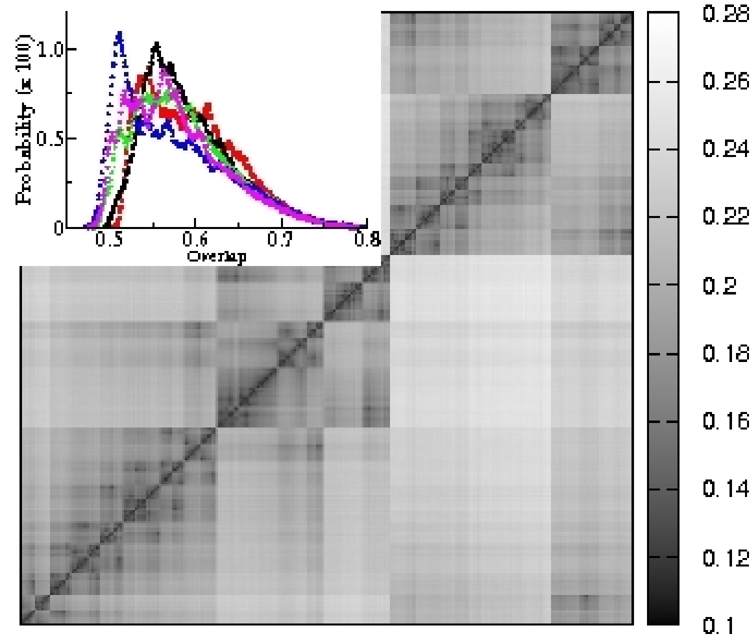


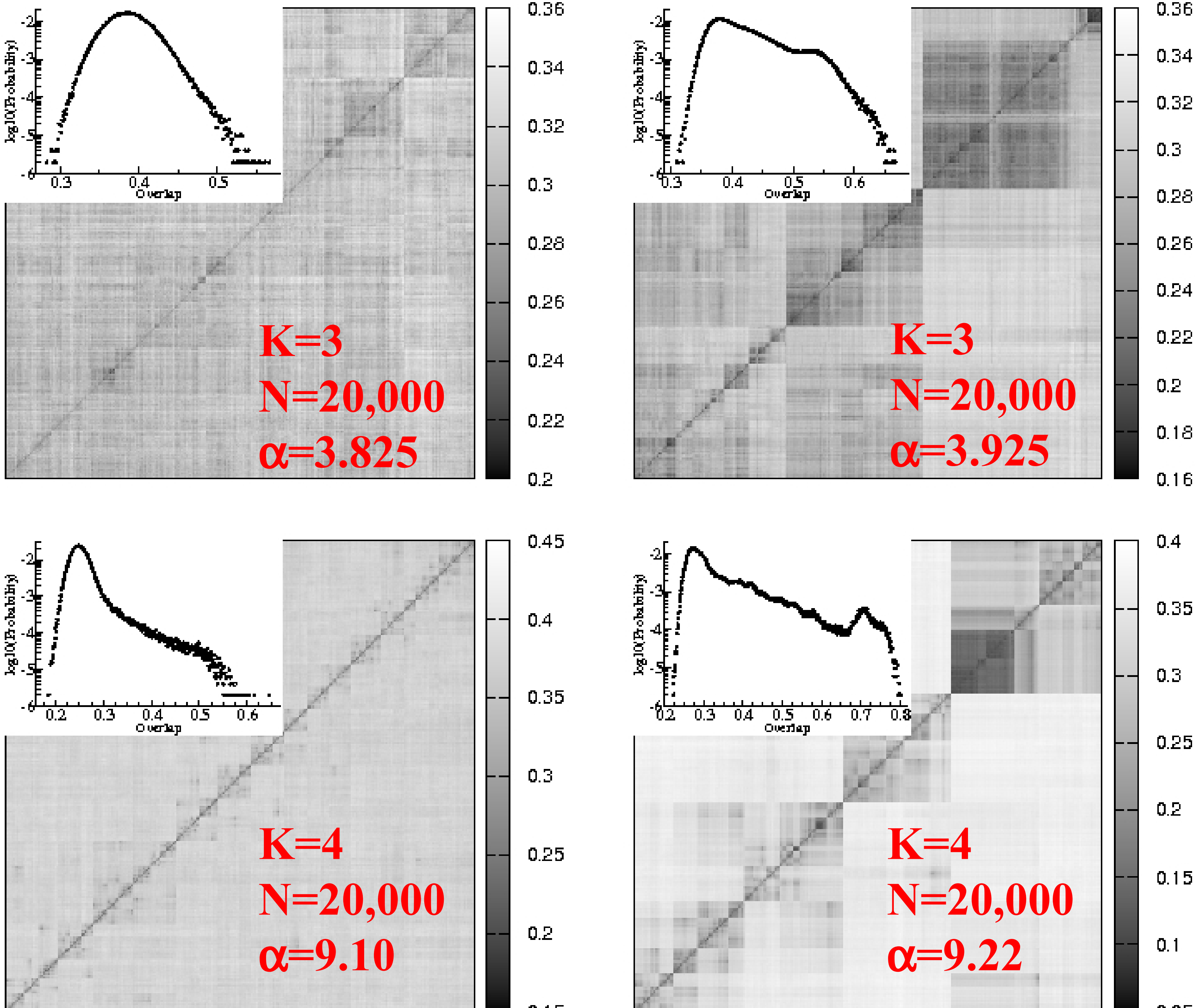
K=4
N=100,000
M=946,000
alpha=9.46

Original formula

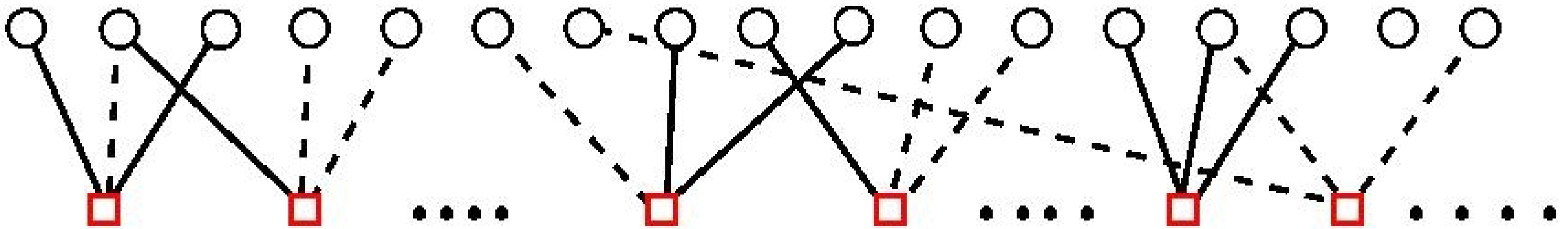


A specially randomized version

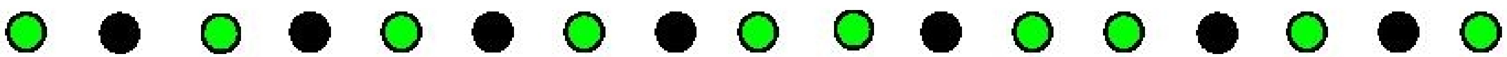



K=3
N=20,000
α=3.825
K=3
N=20,000
α=3.925
K=4
N=20,000
α=9.10
K=4
N=20,000
α=9.22
log10(Probability)
Overlap

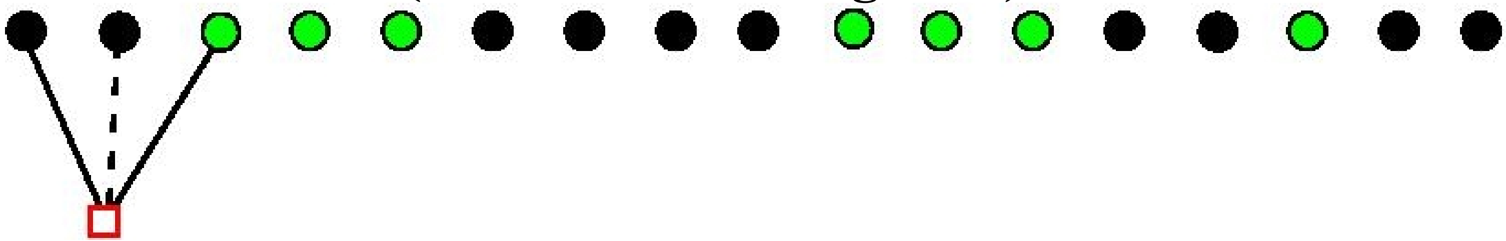
Stochastic search SEQSAT within a solution cluster



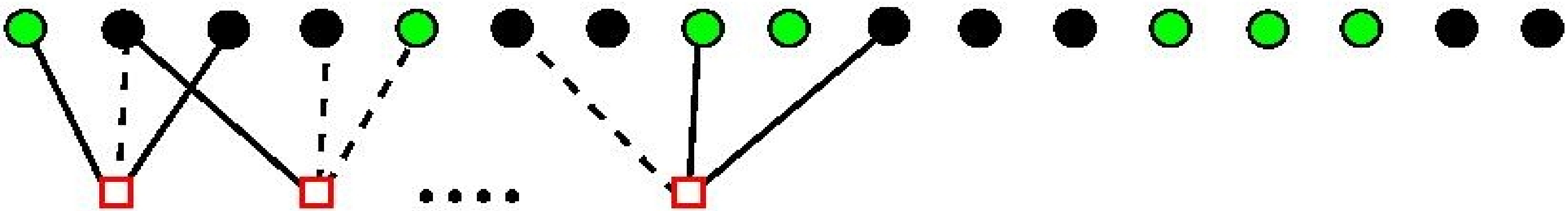
Remove all clauses, randomly generate an initial configuration



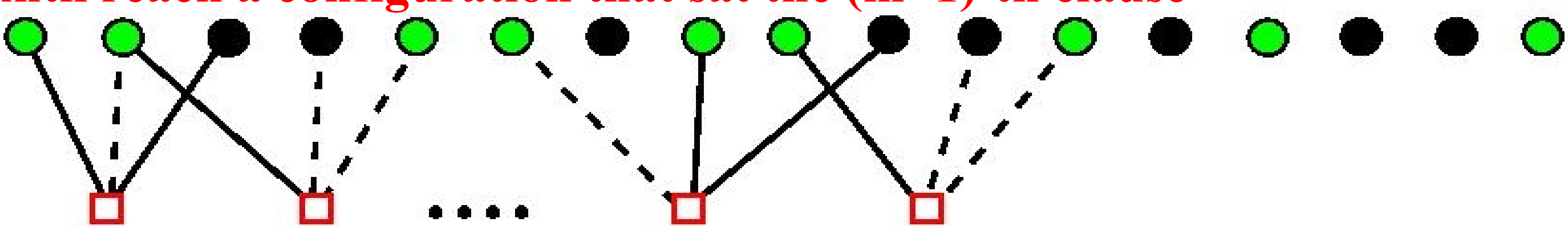
Random walking in the solution cluster until reach a configuration that sat the 1st clause (record the waiting time)



a configuration that sat the first m clauses is reached at certain time



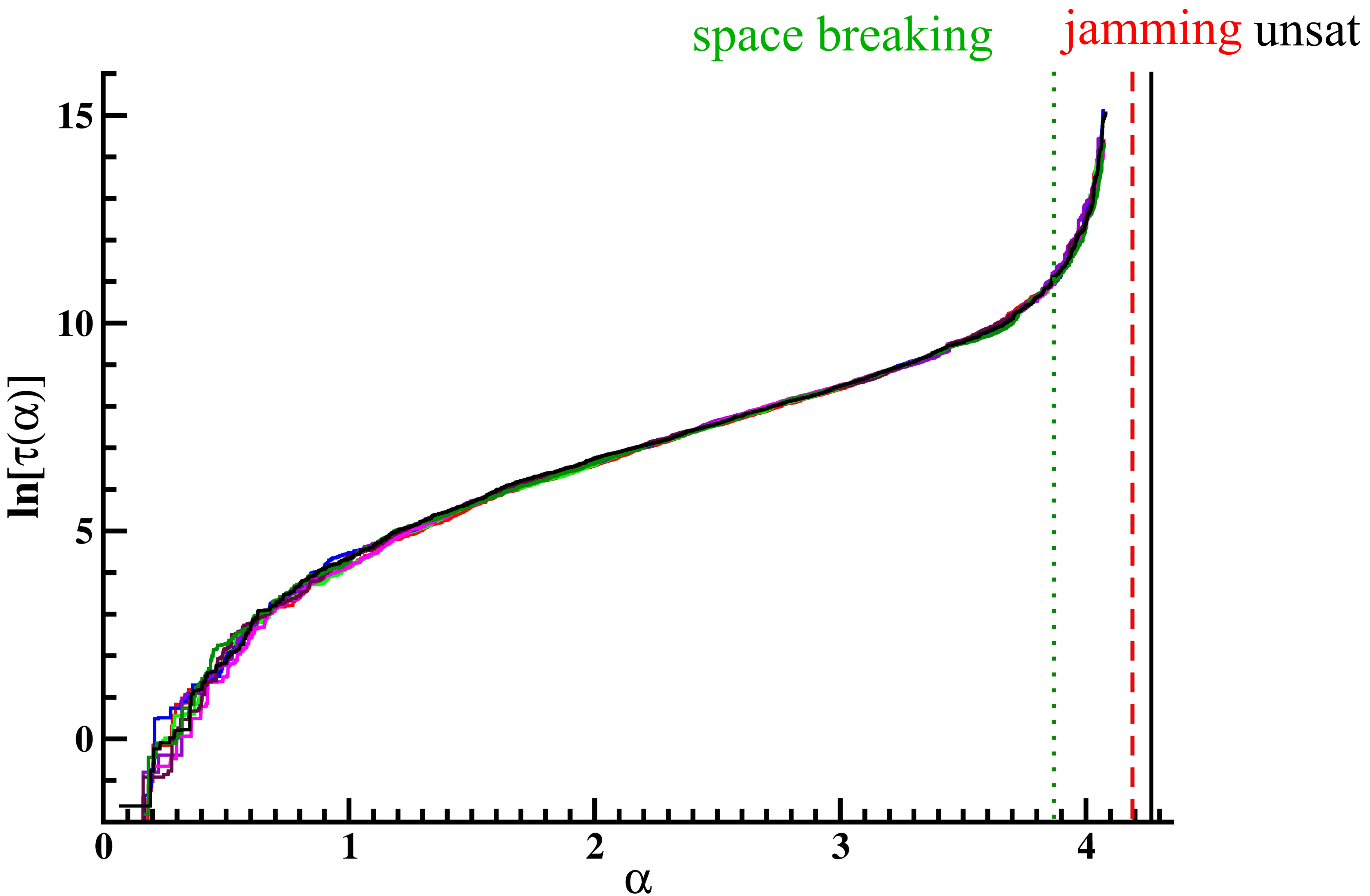
Random walking in the solution cluster of the satisfied subformula
until reach a configuration that sat the (m+1)-th clause



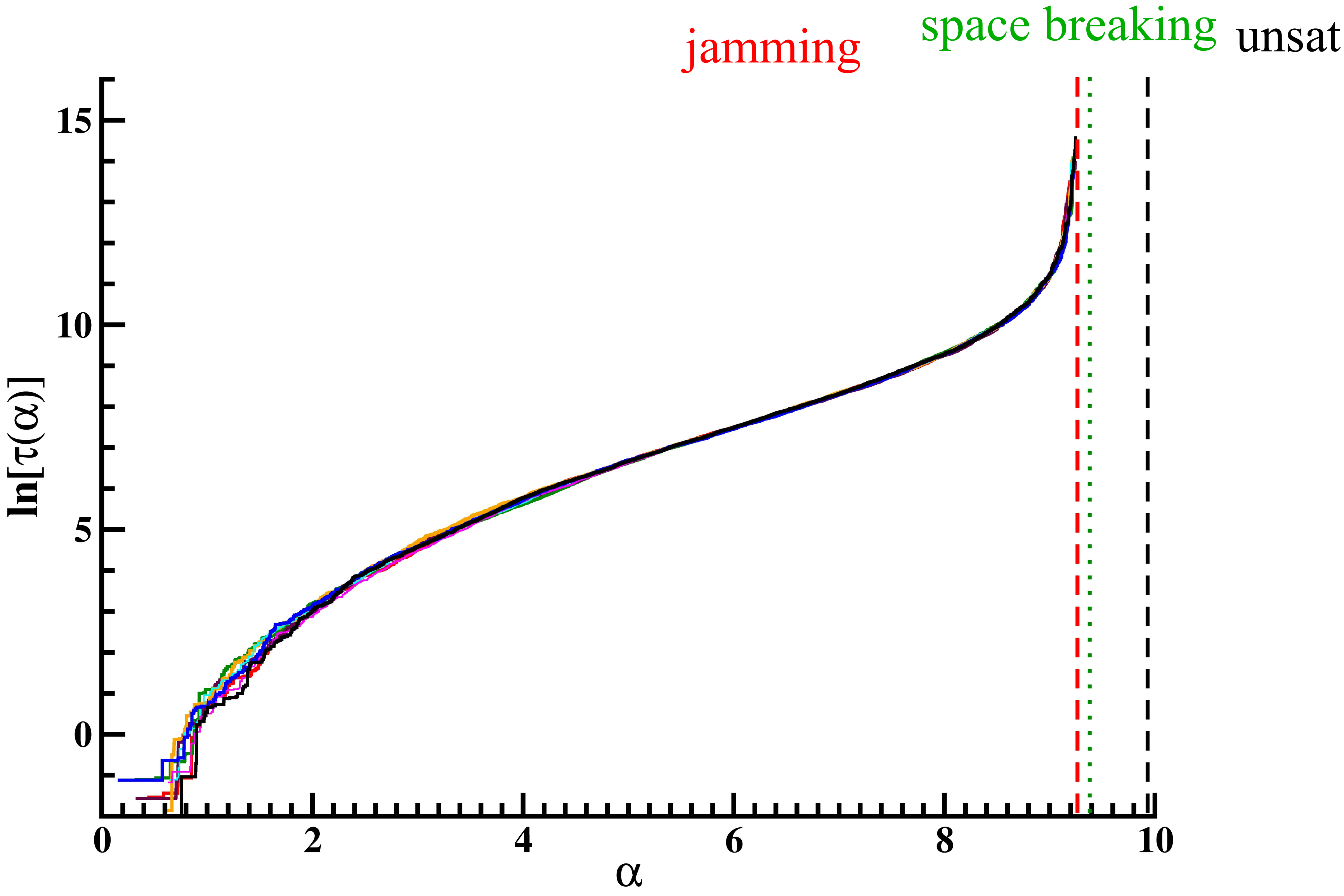
properties of SEQSAT

- never crosses any energy barrier
- never jumps from one solution cluster to another different solution cluster
- just performs random walks within one solution cluster

Performance of SEQSAT: K=3, N=100,000



Performance of SEQSAT: K=4, N=100,000



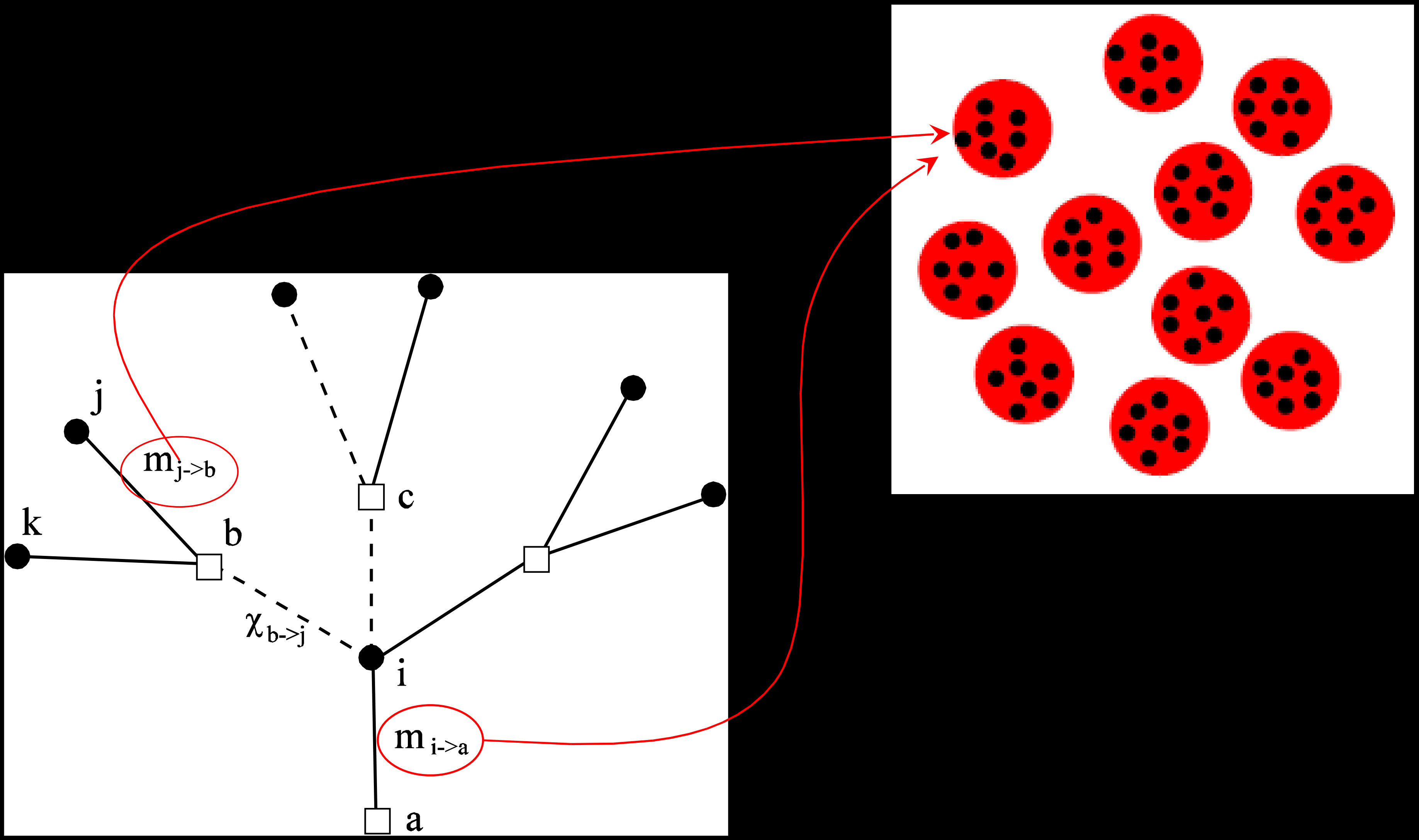
自旋玻璃低温性质的计算机模拟

- 无序样本
- 单个样本的 Monte Carlo 模拟
- 对多个样本的平均

$$\mathcal{H}(\sigma_1, \sigma_2, \ldots, \sigma_N)$$

$$\mathcal{Z} = \sum_{\sigma_1,\ldots,\sigma_N} \exp(-\beta\mathcal{H})$$

$$F(\beta) = -\frac{1}{\beta}\log(\mathcal{Z})$$


j
m j->b
k
b
c
χ b->j
i
m i->a
a

Population Dynamics

On each directed edge i->a and a->i, there is a message.
This message takes different values in different macrostates

$$P_{i\to a}(m_{i\to a}) = \frac{\prod_{b\in\partial i\backslash a}\left[\int \mathrm{d}\chi_{b\to i}\hat{P}_{b\to i}(\chi_{b\to i})\right] e^{-y\Delta F_{i\to a}}\,\delta\left(m_{i\to a} - M(\{\chi_{b\to i} : b\in\partial i\backslash a\})\right)}{\prod_{b\in\partial i\backslash a}\left[\int \mathrm{d}\chi_{b\to i}\hat{P}_{b\to i}(\chi_{b\to i})\right] e^{-y\Delta F_{i\to a}}}$$

$$\hat{P}_{a\to i}(\chi_{a\to i}) = \prod_{j\in\partial a\backslash i}\left[\int \mathrm{d}m_{j\to a} P_{j\to a}(m_{j\to a})\right]\delta\left(\chi_{a\to i} - \prod_{j\in\partial a\backslash i}\frac{(1-J_a^j m_{j\to a})}{2}\right)$$