Phase Transitions in Physics and Computer Science

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Magnetism

- When cold enough, Iron will stay magnetized, and even magnetize spontaneously
- But above a critical temperature, it suddenly ceases to be magnetic
- Interactions between atoms remain the same, but global behavior changes!
- Like water freezing, outbreaks becoming epidemics, opinions changing...

The Ising model

- Lattice (e.g. square) with n sites
- Each has a "spin" $s_i = \pm 1$, "up" or "down"
- Energy is a sum over neighboring pairs:

$$E = -\sum_{ij} s_i s_j$$

- Lowest energy: all up or all down
- Highest energy: checkerboard

Boltzmann Distribution

- At thermodynamic equilibrium, temperature T
- Higher-energy states are less likely:

$$P(s) \sim e^{-E(s)/T}$$

- When $T \to 0$, only lowest energies appear
- When $T \to \infty$, all states are equally likely

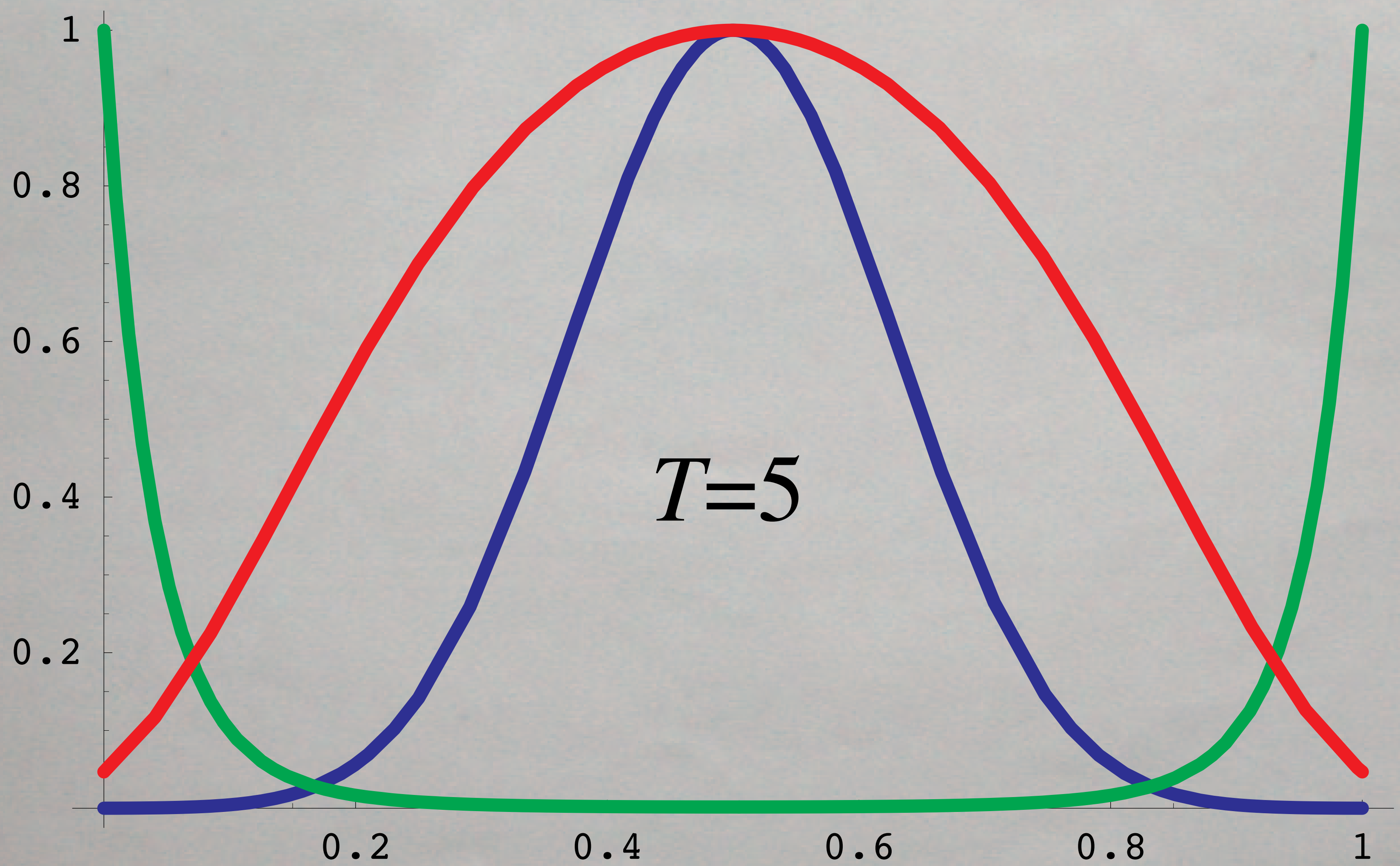
What Happens

- Below critical temperature, the system "magnetizes": mostly up or mostly down
- Small islands of the minority state; as T increases, these islands grow
- Above critical temperature, islands=sea; at large scales, equal numbers of up and down
- When $T=T_c$, islands of all scales: system is scale-invariant!

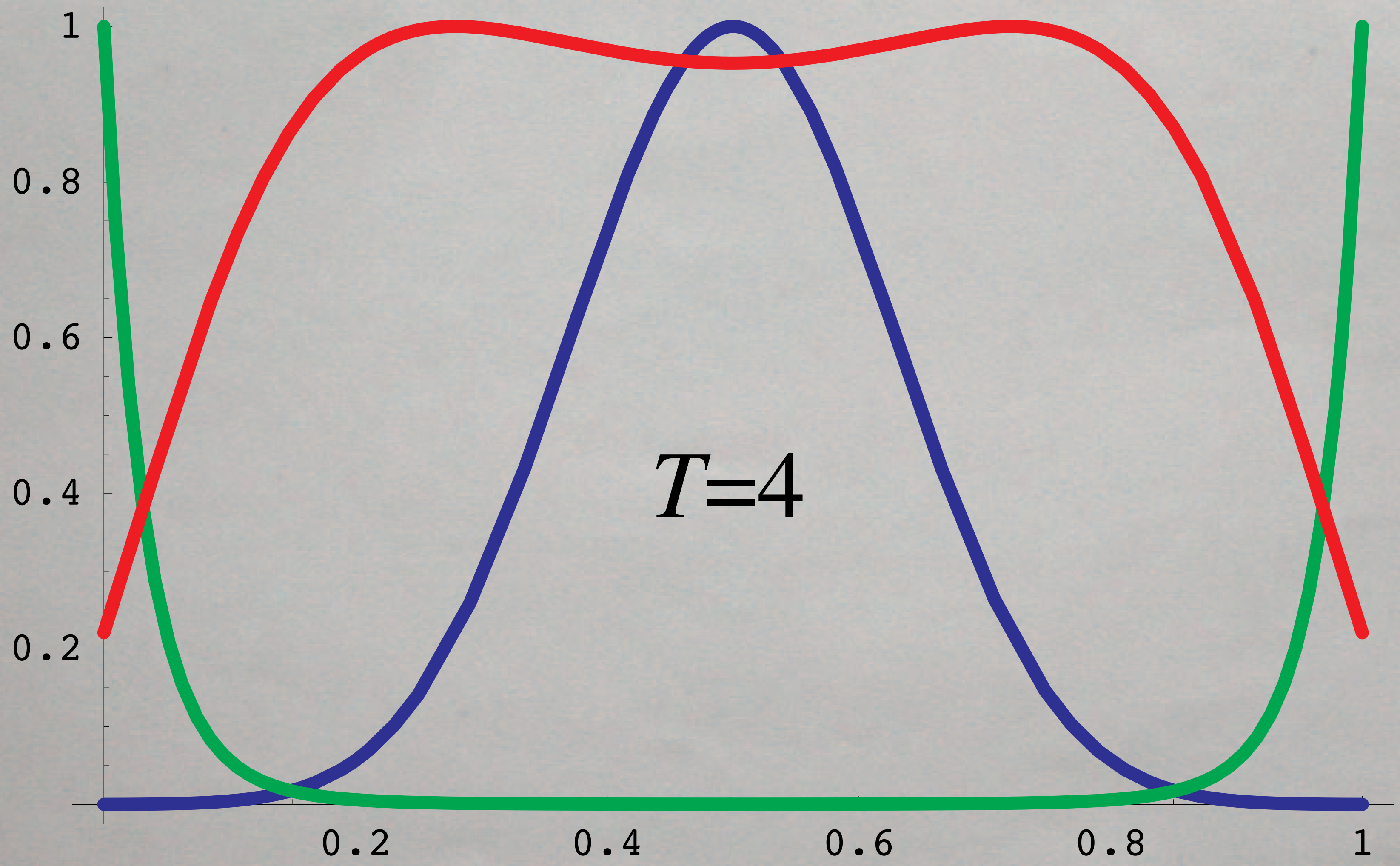
Mean Field

- Ignore topology: forget lattice structure
- If a of the sites are up and $1–a$ are down, energy is $E = 2n^2\left(2a(1-a) - a^2 - (1-a)^2\right)$
- At any T, most-likely states have a=0 or a=1
- But the number of such states is $\binom{n}{an}$, which is tightly peaked around a=1/2.
- Total probability(a) = #states(a) Boltzmann(a)

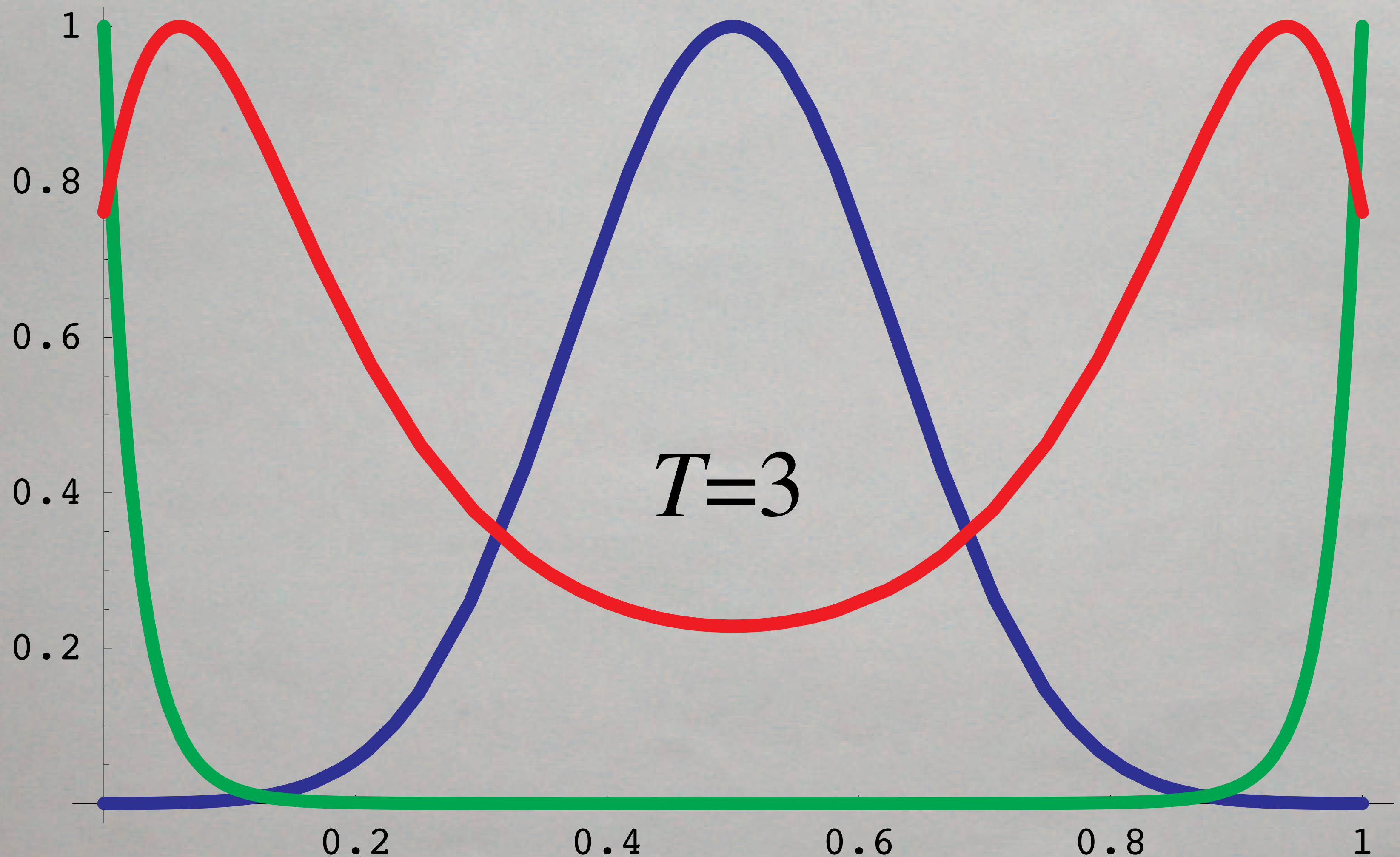
Energy vs. Entropy



Energy vs. Entropy



Energy vs. Entropy



Correlations

- $C(r)$ = correlation between two sites r apart
- If $T > T_c$, correlations decay exponentially:

$$C(r) \sim e^{-r/\ell}$$

- Correlation length ℓ decreases as T grows
- As we approach T_c, correlation length diverges
- At T_c, power-law correlations (scale-free):

$$C(r) \sim \ell^{-\alpha}$$

Percolation

- Fill a fraction p of the sites in a lattice
- When $p < p_c$, small islands, whose size is exponentially distributed:

$$P(s) \sim e^{-s/\overline{s}}$$

- When $p > p_c$, "giant cluster" appears
- At p_c, power-law distribution of cluster sizes:

$$P(s) \sim s^{-\alpha}$$

The Adversary

...designs problems that are as diabolically hard as possible, forcing us to solve them in the worst case. (Hated and feared by computer scientists.)

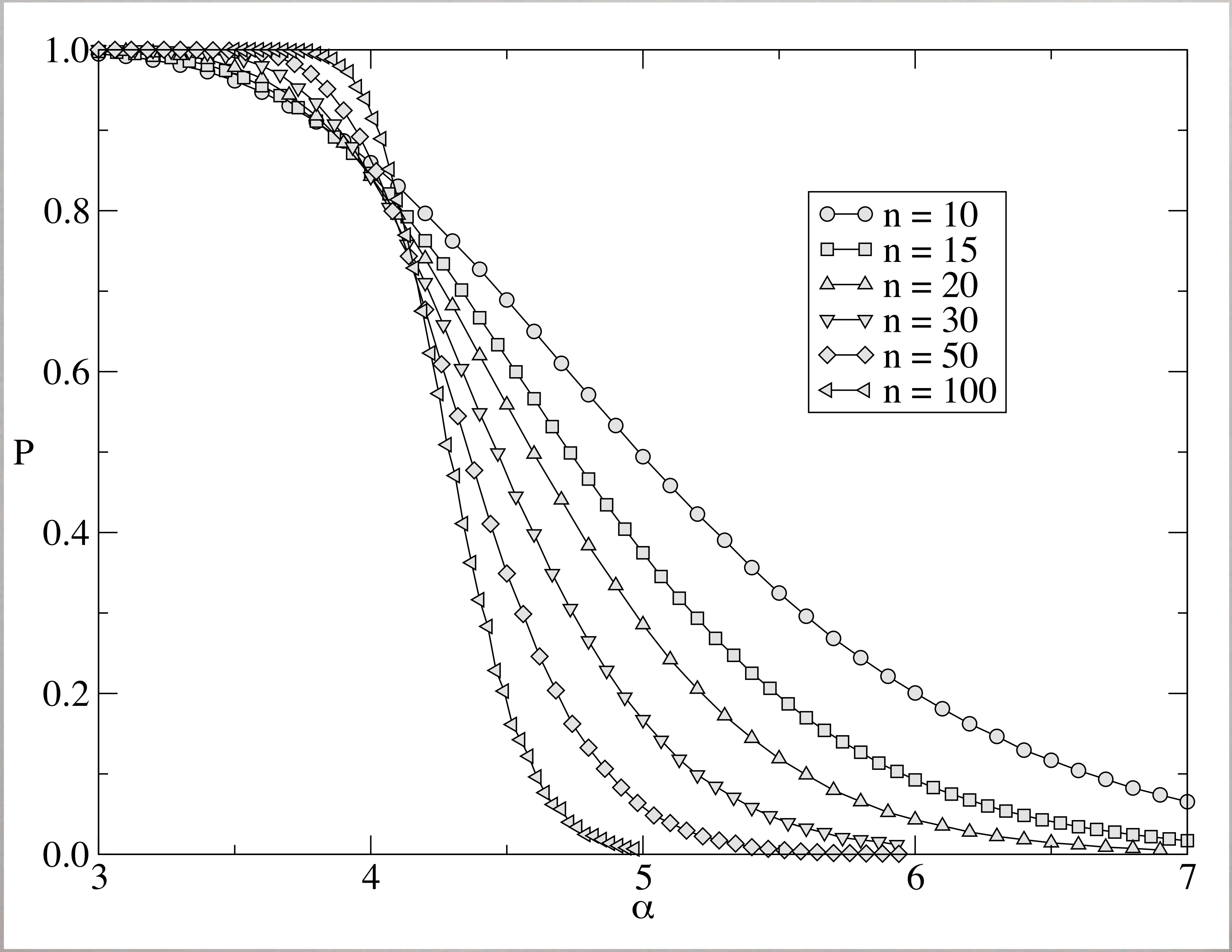
La Dame Nature

...asks questions whose answers are simpler and more beautiful than we have any right to imagine. (Worshipped by physicists.)

Random NP Problems

- A 3-SAT formula with n variables, m clauses
- Choose each clause randomly: $\binom{n}{3}$ possible triplets, negate each one with probability 1/2
- Precedents:
  - Random Graphs (Erdős-Rényi)
  - Statistical Physics: ensembles of disordered systems, e.g. spin glasses
- Sparse Case: $m = \alpha n$ for some density α

A Phase Transition



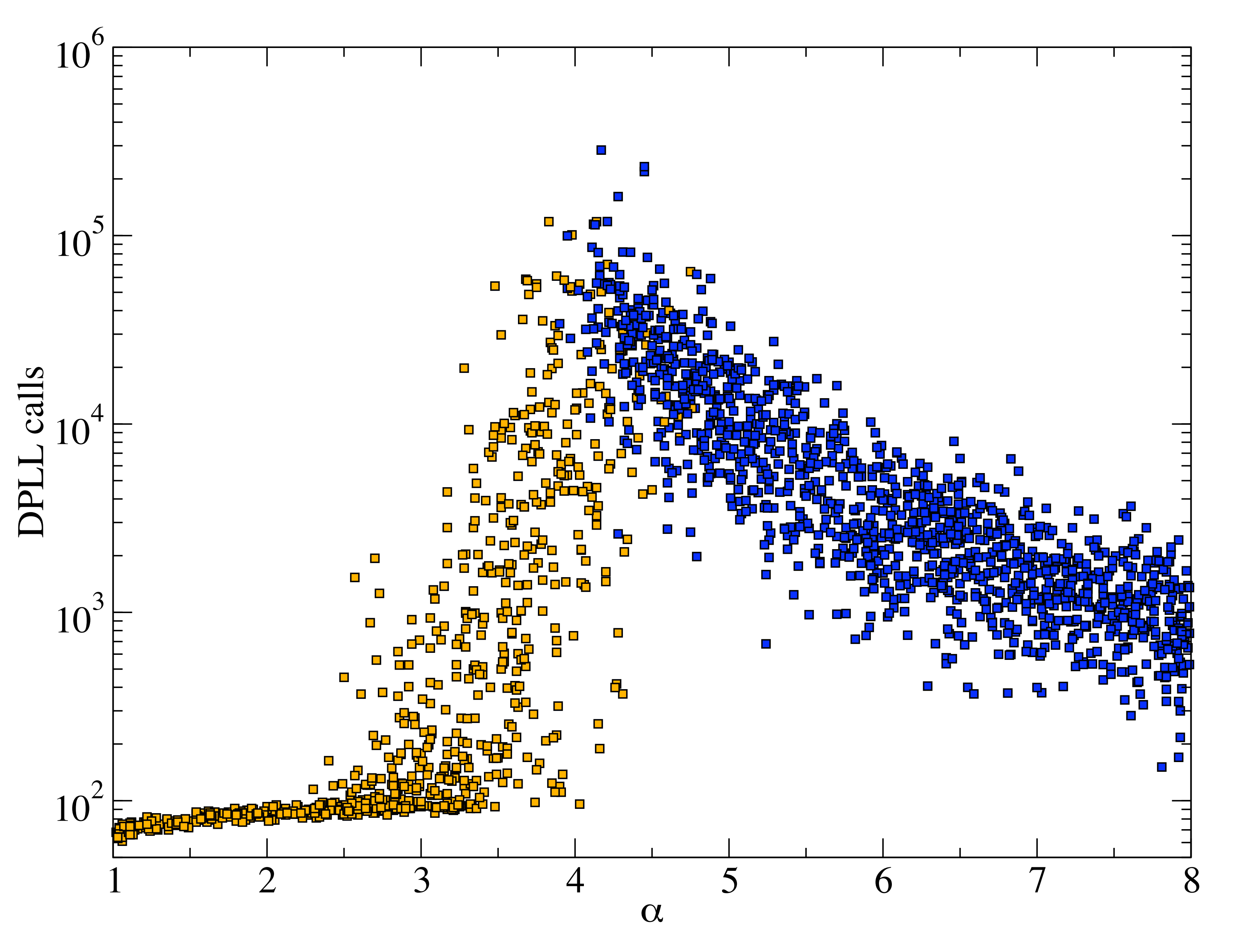
The Threshold Conjecture

- We believe that for each $k \geq 3$, there is a critical clause density α_k such that

$$\lim_{n \to \infty} \Pr\left[F_k(n, m = \alpha n) \text{ is satisfiable}\right] = \begin{cases} 1 & \text{if } \alpha < \alpha_k \\ 0 & \text{if } \alpha > \alpha_k \end{cases}$$

- So far, only known rigorously for $k = 2$

Search Times



An Upper Bound

- The *average* number of solutions $\mathrm{E}[X]$ is

$$2^n \left(\frac{7}{8}\right)^m = \left(2\left(\frac{7}{8}\right)^\alpha\right)^n$$

- This is exponentially small whenever

$$\alpha > \log_{8/7} 2 \approx 5.19$$

- But the transition is much lower, at $\alpha \approx 4.27$. What's going on?

A Heavy Tail

- In the range $4.27 < \alpha < 5.19$, the average number of solutions is exponentially large.
- Occasionally, there are exponentially many...
- ...but most of the time there are none!
- A classic "heavy-tailed" distribution
- Large average doesn't prove satisfiability!

Lower Bound #1

- Idea: track the progress of a simple algorithm!
- When we set variables, clauses disappear or get shorter:

$$\overline{x} \wedge (x \vee y \vee z) \Rightarrow (y \vee z)$$

- *Unit Clauses* propagate:

$$x \wedge (\overline{x} \vee y) \Rightarrow y$$

One Path Through the Tree

- If there is a unit clause, satisfy it. Otherwise, choose a random variable and give it a random value!

- The remaining formula is random for all *t*:

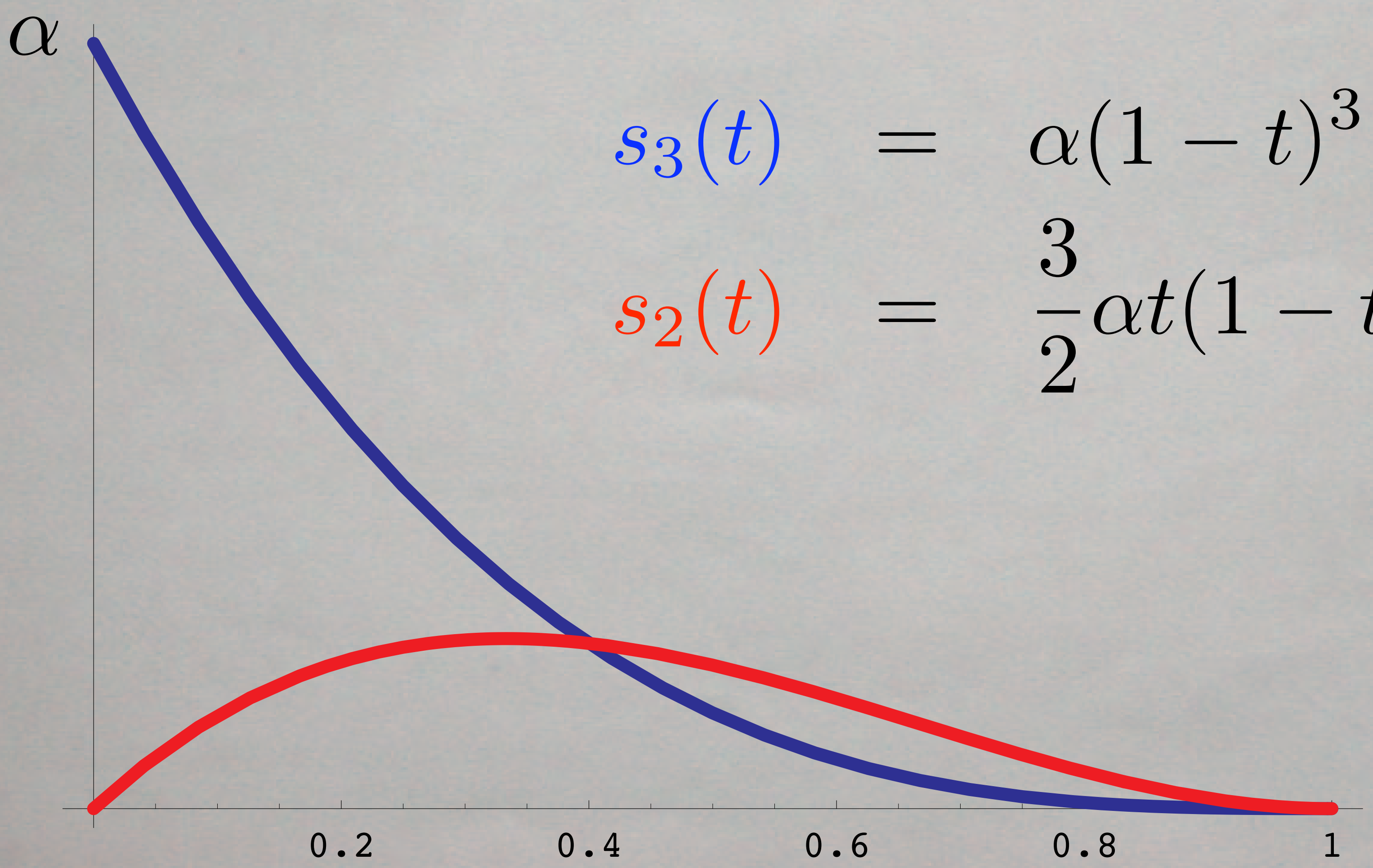
$$\frac{ds_3}{dt} = -\frac{3s_3}{1-t} \; , \qquad \frac{ds_2}{dt} = \frac{(3/2)s_3 - 2s_2}{1-t}$$

$$s_3(0) = \alpha \; , \quad s_2(0) = 0$$

One Path Through the Tree

- These differential equations give

$$
\begin{aligned}
{\color{blue}s_3(t)} &= \alpha(1-t)^3 \\
{\color{red}s_2(t)} &= \frac{3}{2}\alpha t(1-t)^2
\end{aligned}
$$



Branching Unit Clauses

- Each unit clause has on average λ children, where

$$\lambda = \frac{1}{2}\frac{2s_2}{1-t} = \frac{3}{4}\alpha t(1-t)$$

- When $\lambda > 1$, they proliferate and contradictions appear
- Maximized at $t = 1/2$
- But if $\alpha < 8/3$, then $\lambda < 1$ always, and the unit clauses stay manageable.

Constructive Methods Fail

- Fancier algorithms, harder math: $\alpha < 3.52$.
- But, for larger k, algorithmic methods are nowhere near the upper bound for k-SAT:

$$O\left(\frac{2^k}{k}\right) < \alpha < O(2^k)$$

- To close this gap, we need to resort to non-constructive methods.

Lower Bound #2

- Idea: bound the *variance* of the number of solutions.
- If X is a nonnegative random variable,

$$\Pr[X > 0] \geq \frac{\mathrm{E}[X]^2}{\mathrm{E}[X^2]}$$

- $\mathrm{E}[X]$ is easy; $\mathrm{E}[X^2]$ requires us to understand *correlations* between solutions.

Correlations

- The second moment $\mathrm{E}[X^2]$ is the expected number of *pairs* of satisfying assignments.

- If two assignments have *overlap* z, they satisfy a random *k*-SAT clause with probability

$$q(z) = 1 - 2 \cdot 2^{-k} + z^k 2^{-k}$$

- Note that

$$q(1/2) = (1 - 2^{-k})^2$$

as if the pair were independent.

Correlations

- Now $\mathrm{E}[X^2]$ is the number of pairs with overlap z, times the probability each pair is satisfying, summed over z:

$$\mathrm{E}[X^2] \approx \sum_z 2^n \binom{n}{zn} q(z)^{\alpha n} dz$$

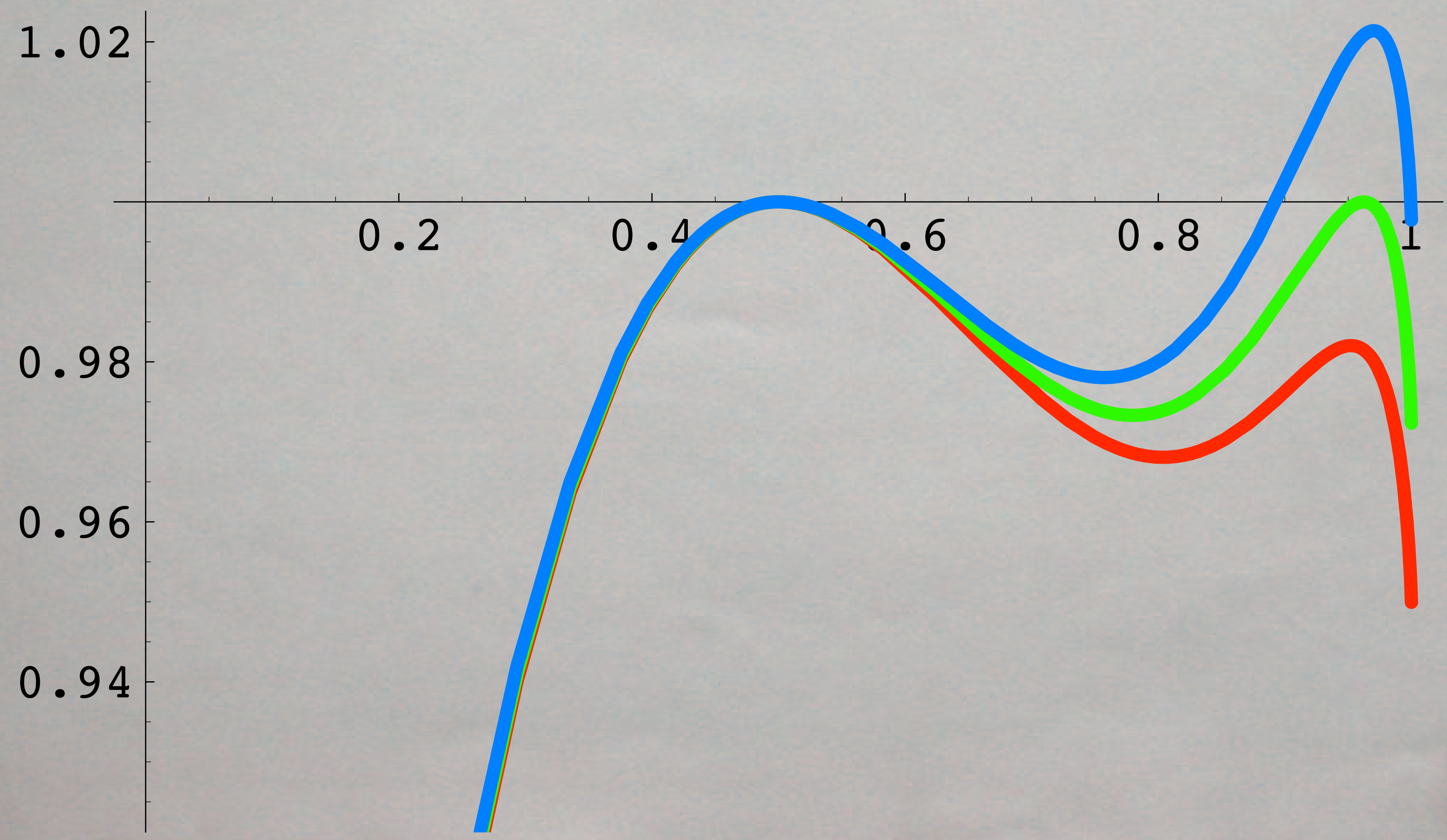
$$\approx 2^n \int_0^1 e^{n\left(h(z)+\alpha \ln q(z)\right)} dz$$

where $h(z) = -z \ln z - (1-z)\ln(1-z)$

- Again, a tradeoff between entropy and "energy."

A Function of Distance

- When the expected number of *pairs* of solutions is peaked at 1/2, most pairs are "independent" and the variance is small.



Determining the Threshold

- A series of results has narrowed the range for the transition in k-SAT to

$$2^k \ln 2 - O(k) < \alpha < 2^k \ln 2 - O(1)$$

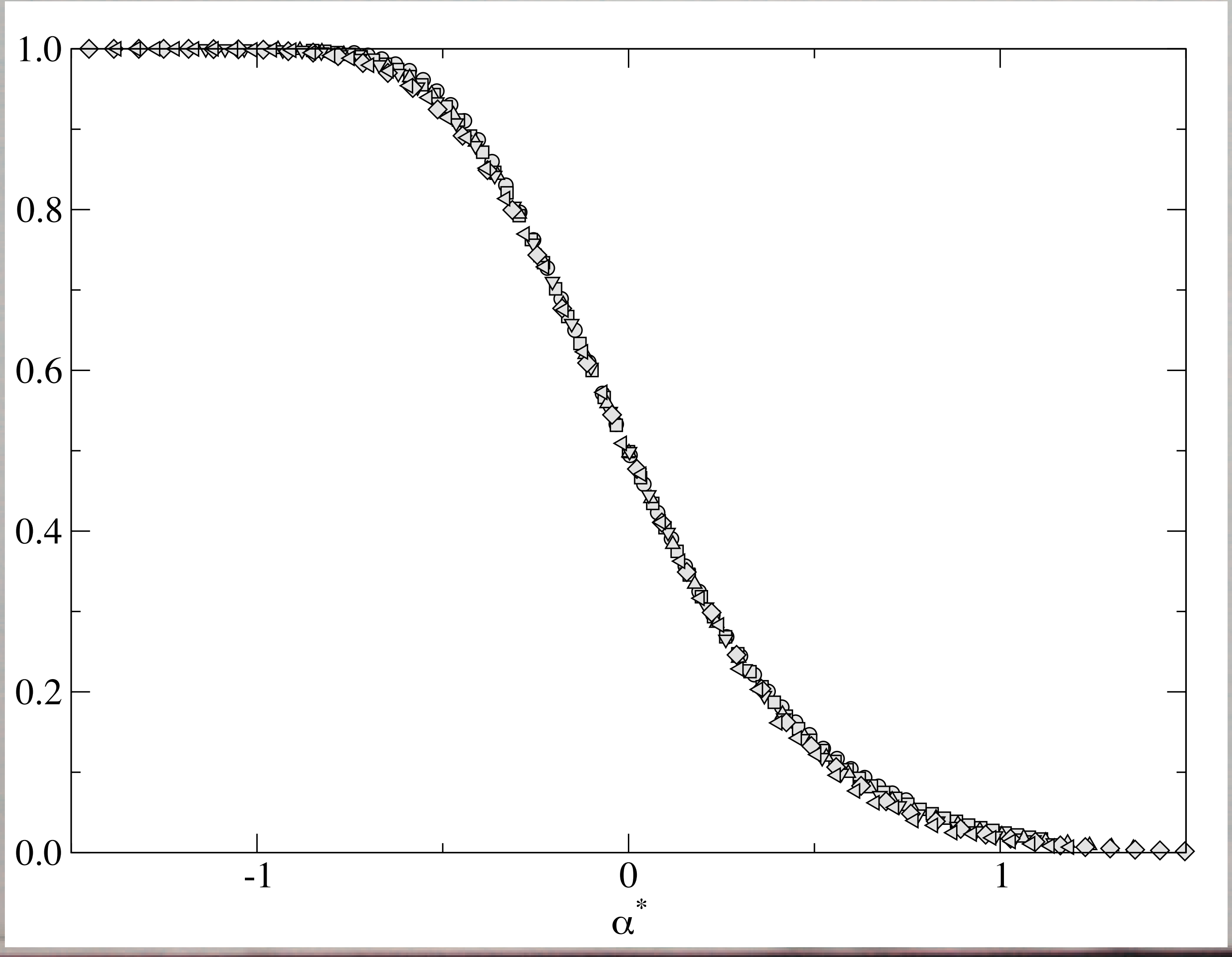
- Prediction from statistical physics:

$$2^k \ln 2 - O(1)$$

- Seems difficult to prove with current methods.

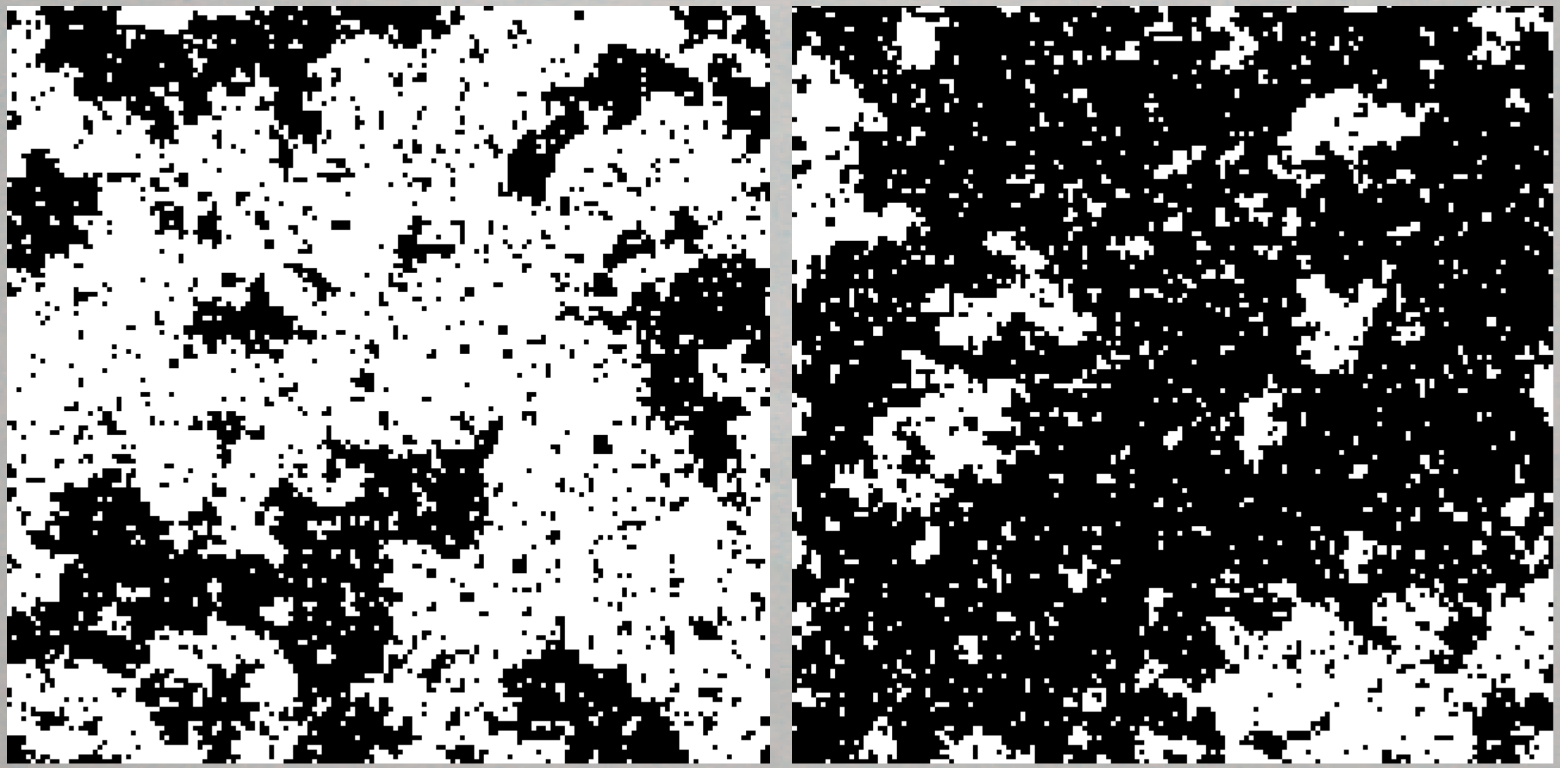
Scaling and Universality

- Rescaling α around the critical point causes different n to coincide. A universal function?



Clustering

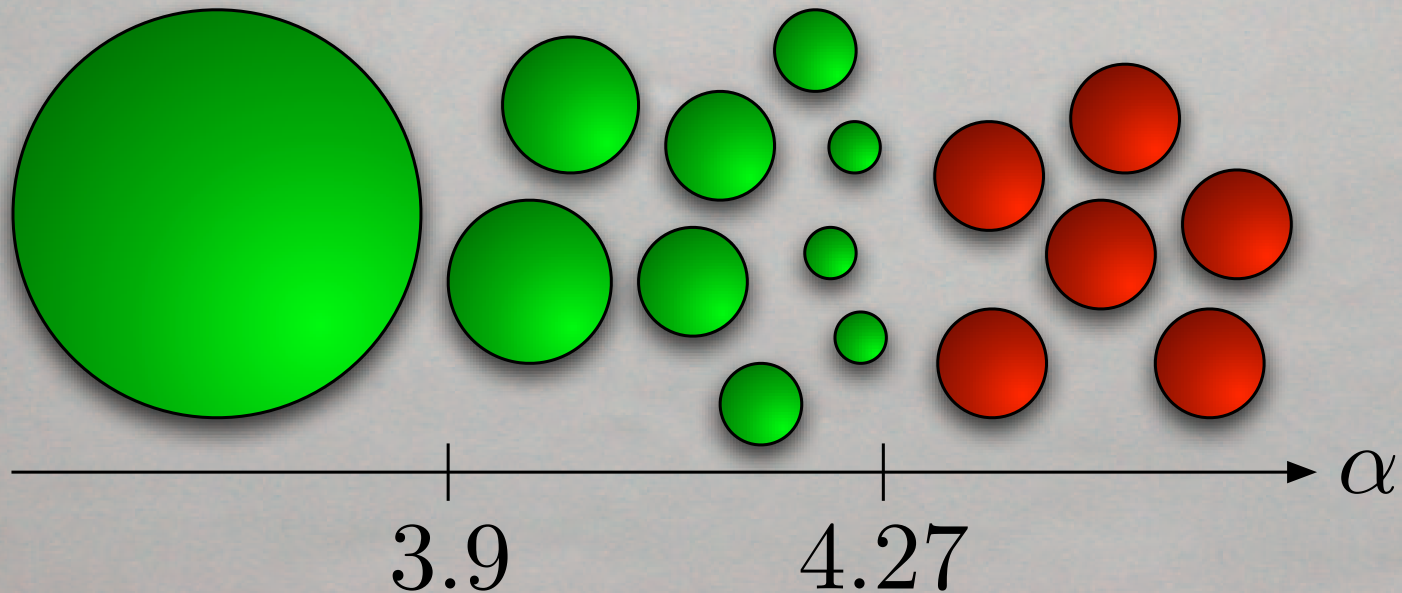
- Below the critical temperature, magnets have two *macrostates* (Gibbs measures)



- Glasses, and 3-SAT, have exponentially many!

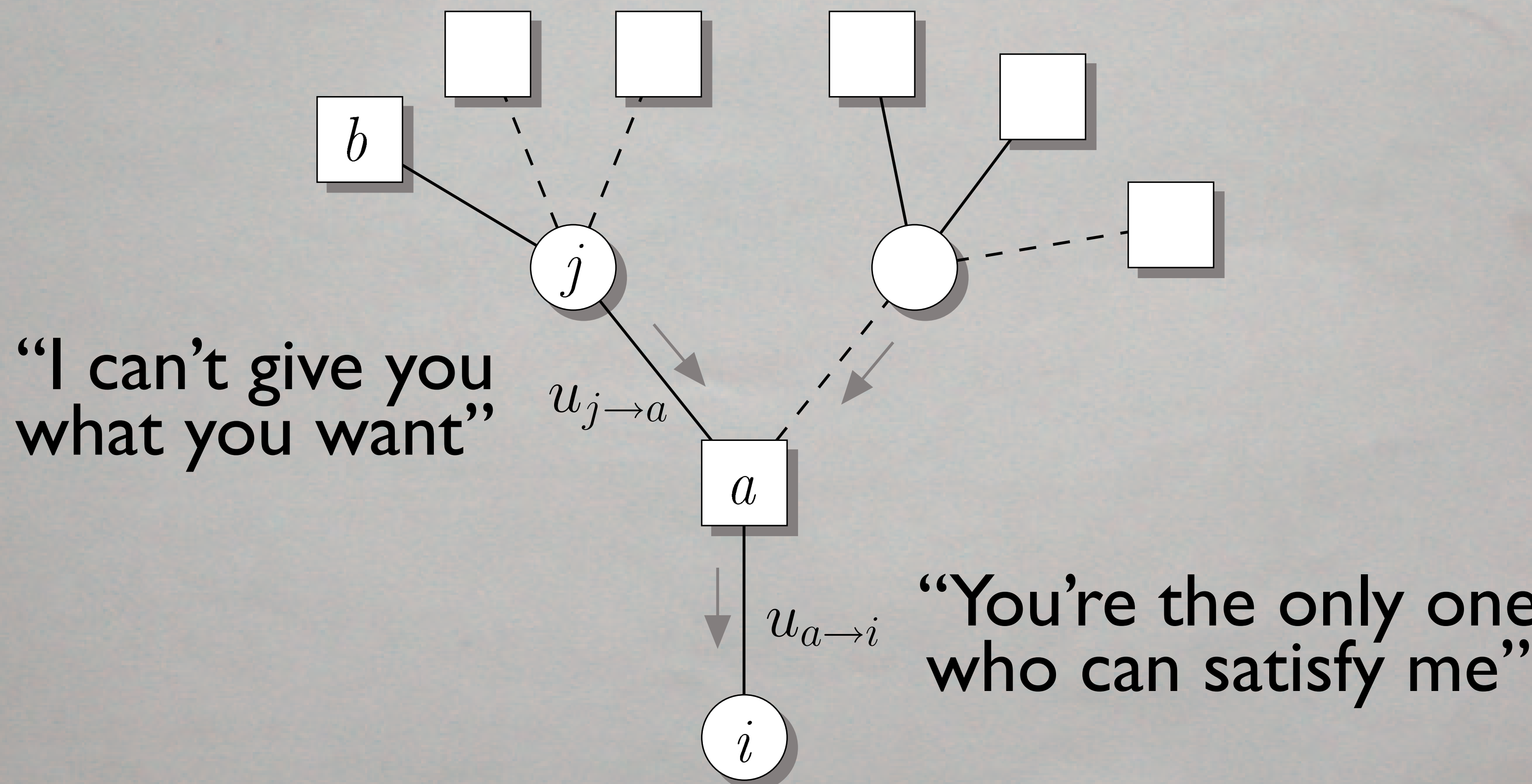
Clustering

- An idea from statistical physics: there is another transition, from a unified "cloud" of solutions to separate clusters.
- Is this why algorithms fail at $\alpha \sim 2^k/k$?



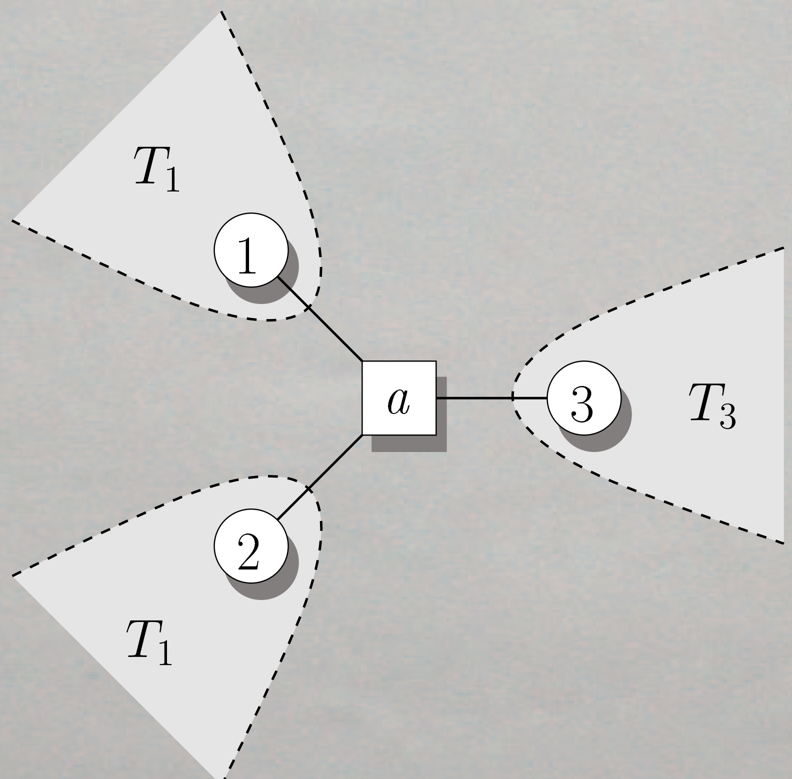
The Physicists' Algorithm

- A "message-passing" algorithm:



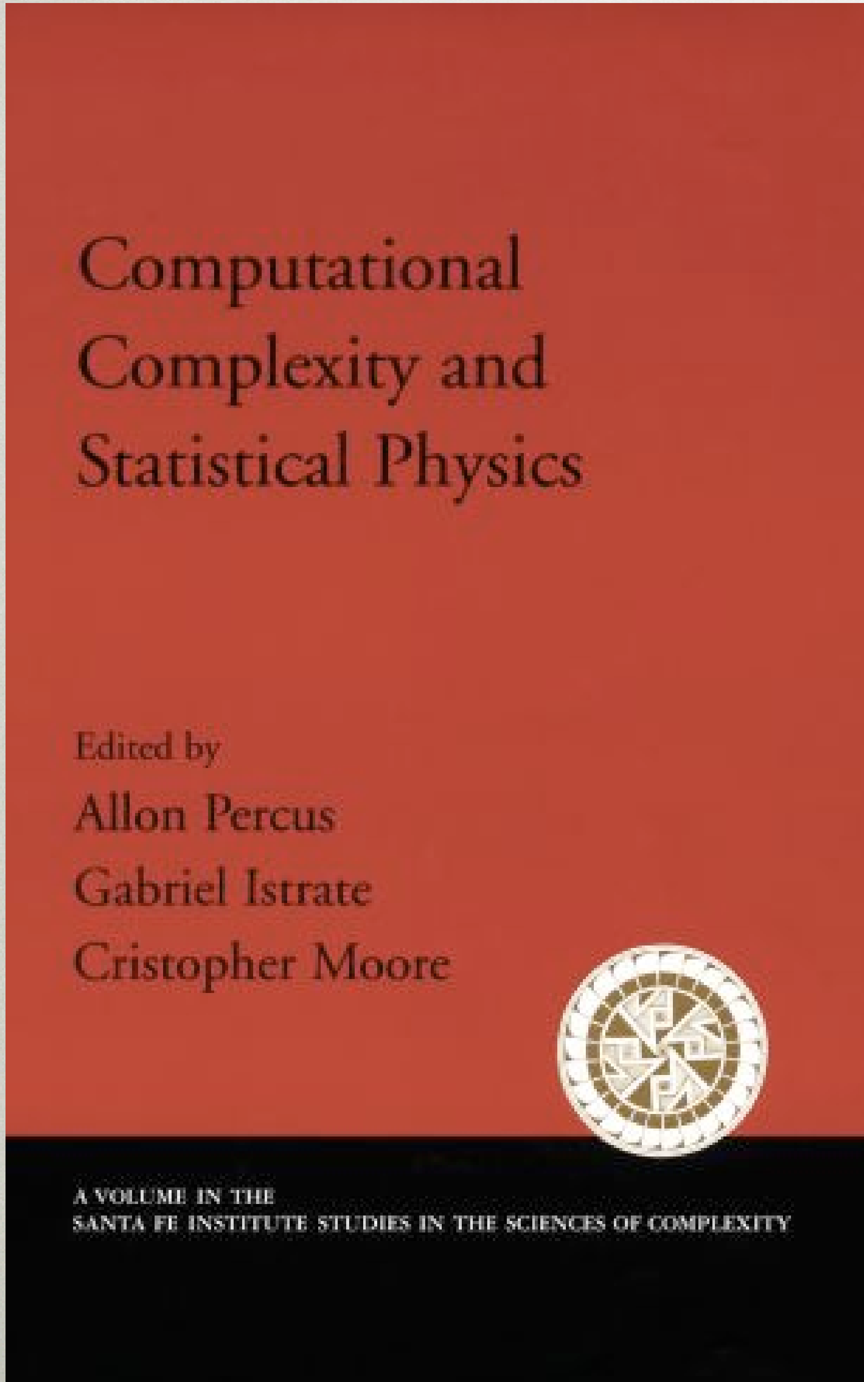
Why Does It Work?

- Random formulas are locally treelike.
- Assume the neighbors are independent:



- *Proving* this will take some very deep work.

Shameless Plugs



Acknowledgments