Phase Transitions in Physics and Computer Science

Cristopher Moore
University of New Mexico
and the Santa Fe Institute

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

640x640 Ising model

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

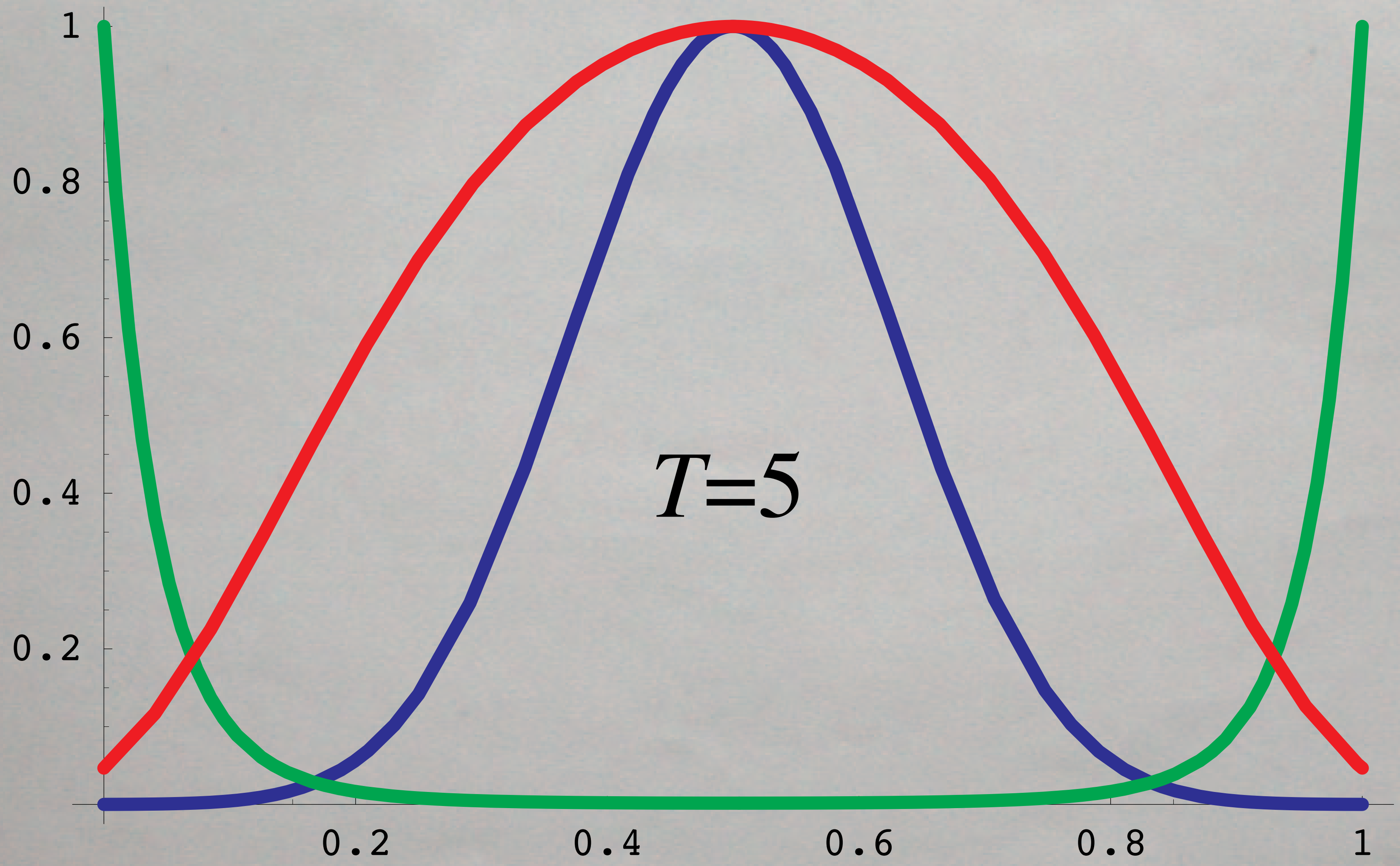
What Happens

- 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!

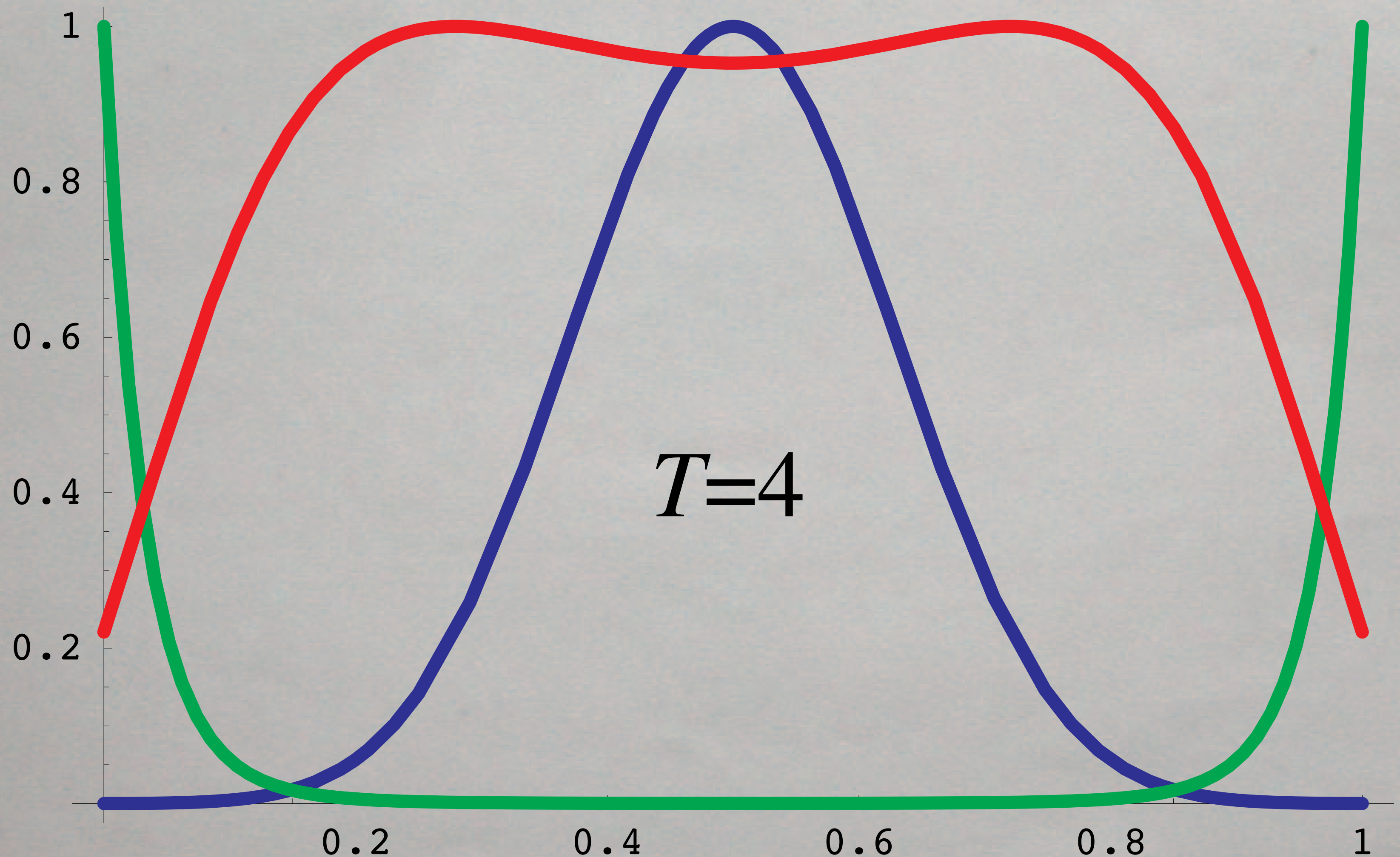
Mean Field

- 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)

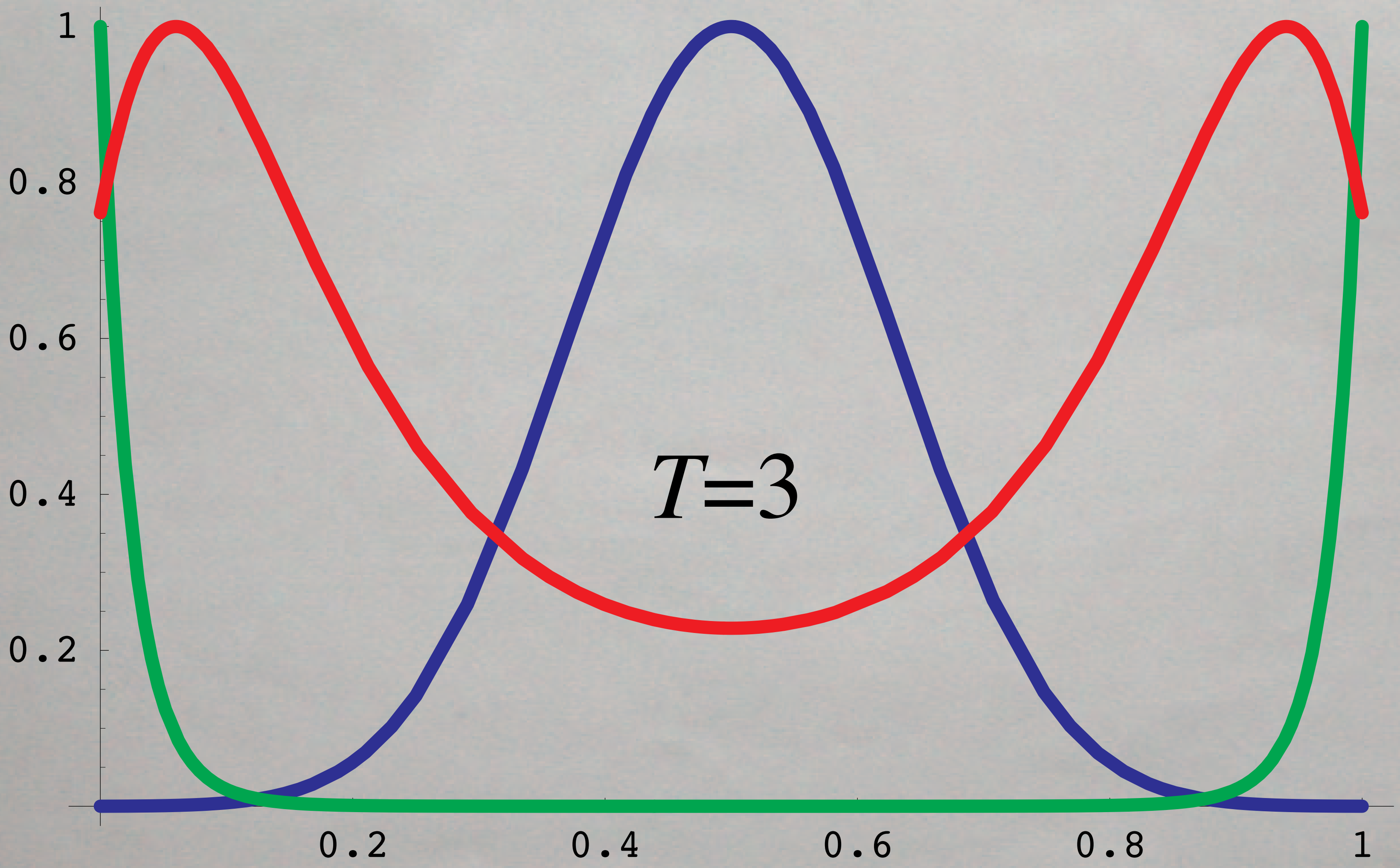
Energy vs. Entropy



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:

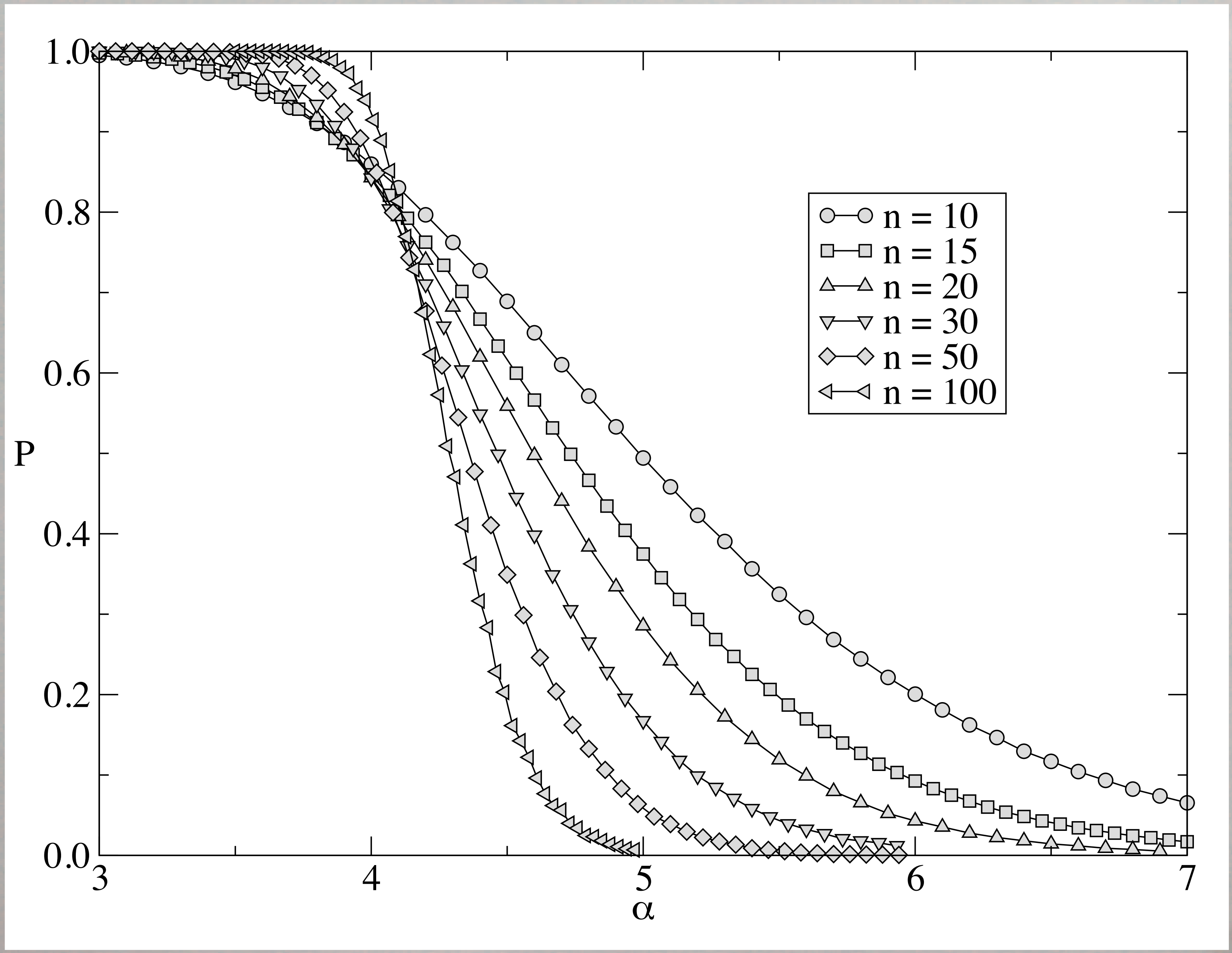
$$P(s) \sim s^{-\alpha}$$

- PHY 411/506 Java Applet: Percolation

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



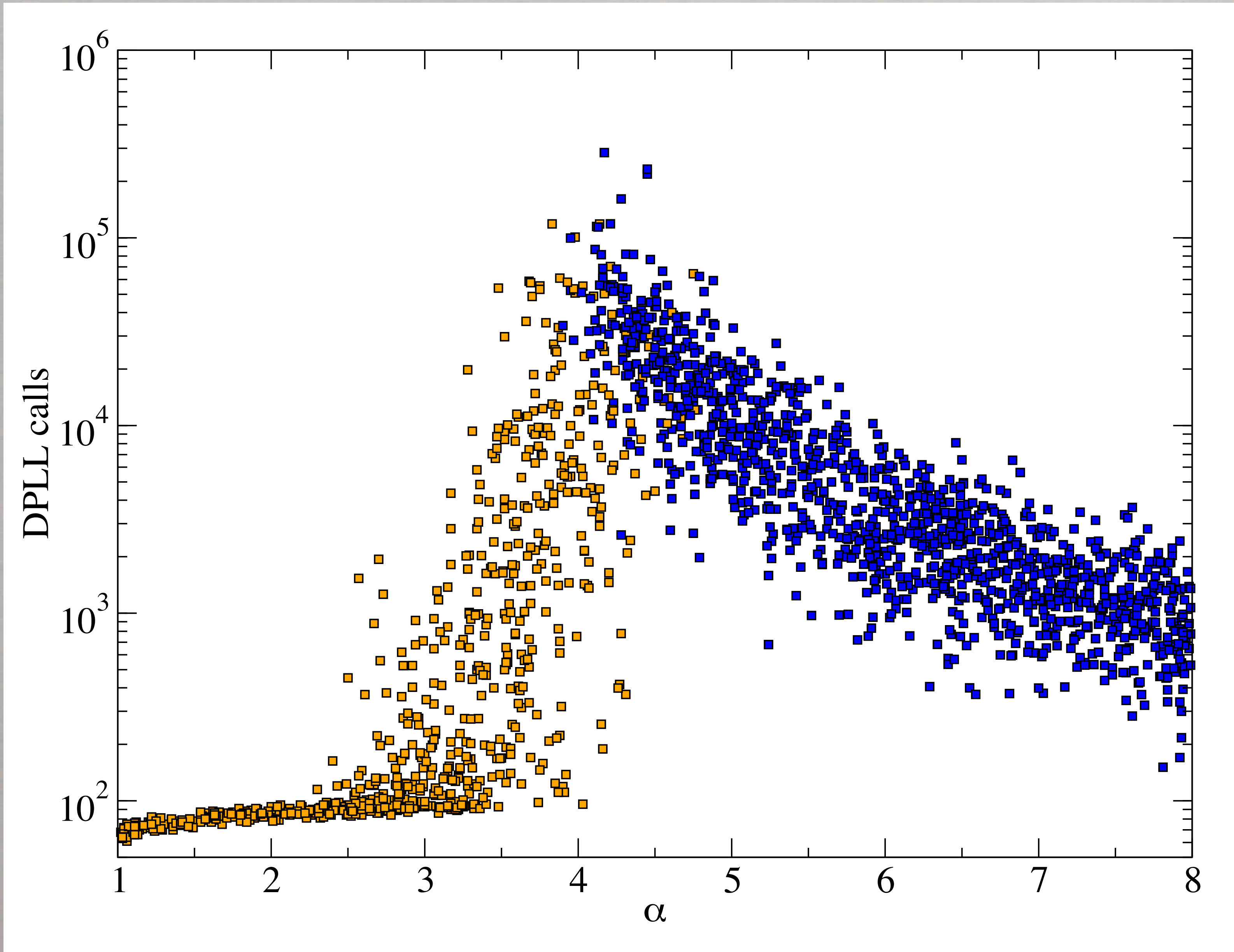
The Threshold Conjecture

- 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

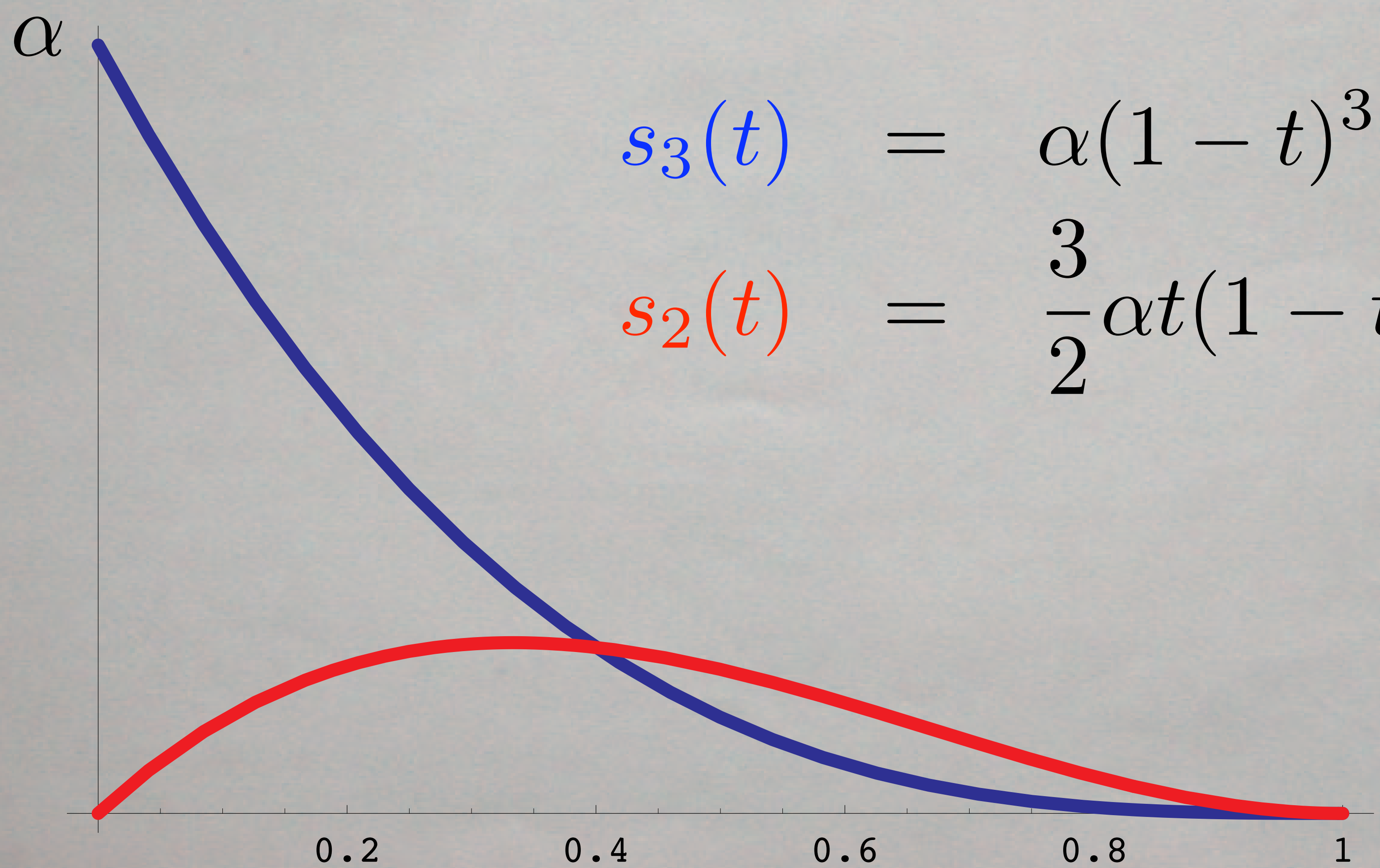
- If there is a unit clause, satisfy it. Otherwise, choose a random variable and give it a random value!
- The remaining formula is random for all *t*:

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

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

One Path Through the Tree

- These differential equations give



$$s_3(t) = \alpha(1-t)^3$$

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

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

- 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.
- Nonconstructive! Doesn't help us find solutions.

Determining the Threshold

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

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

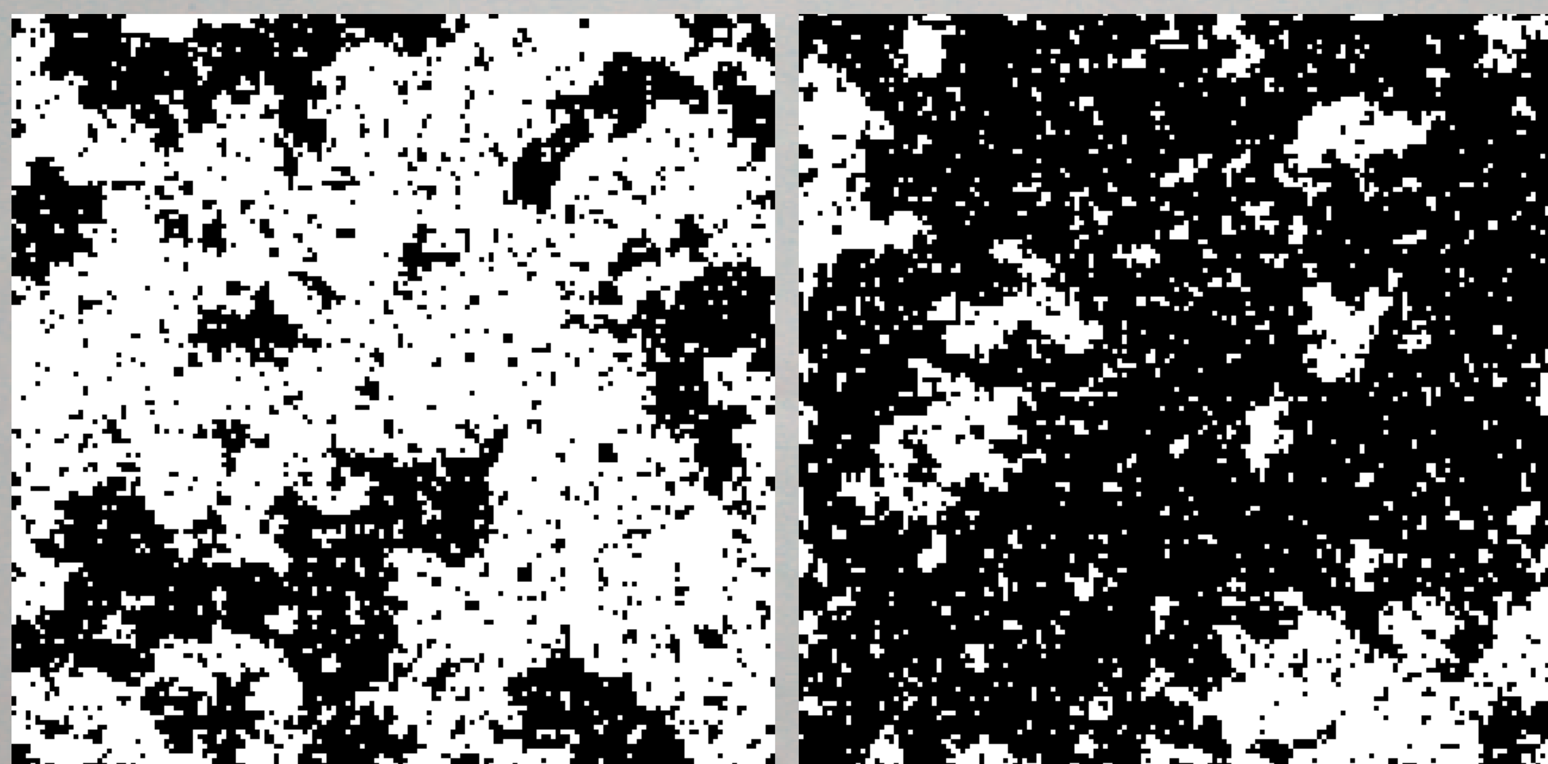
- Prediction from statistical physics:

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

- Seems difficult to prove with current methods.

Clustering

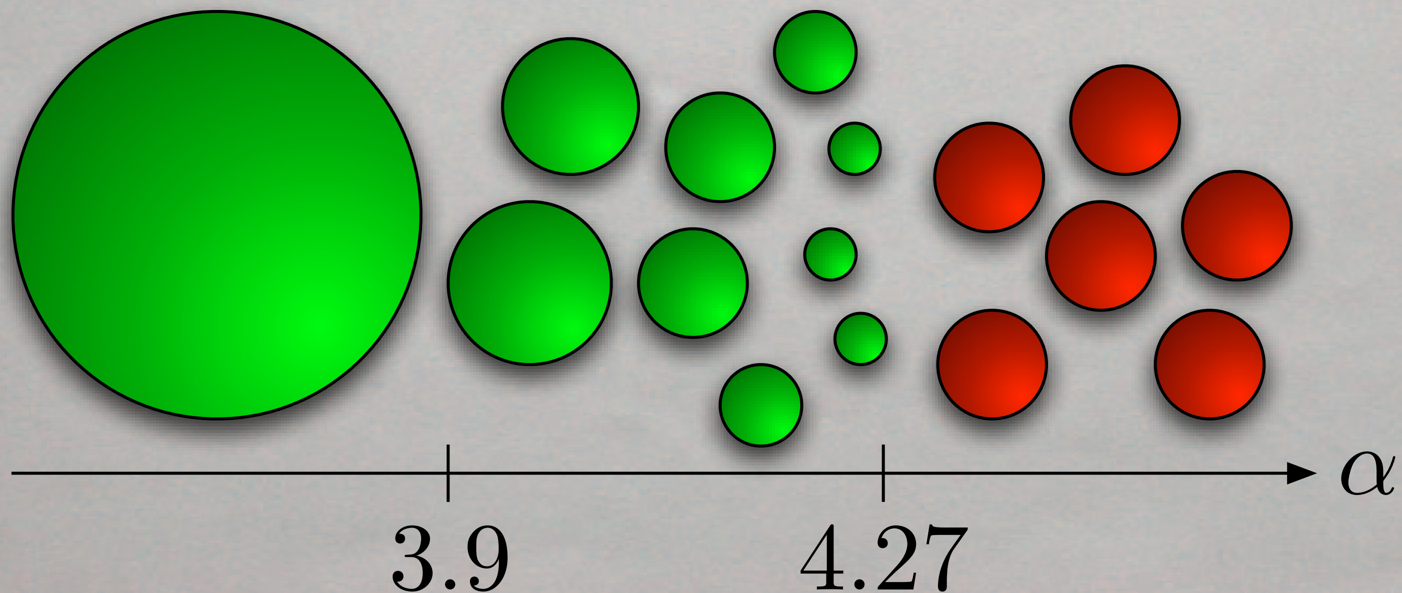
- Below the critical temperature, magnets have two *macrostates* (Gibbs measures)



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

Clustering

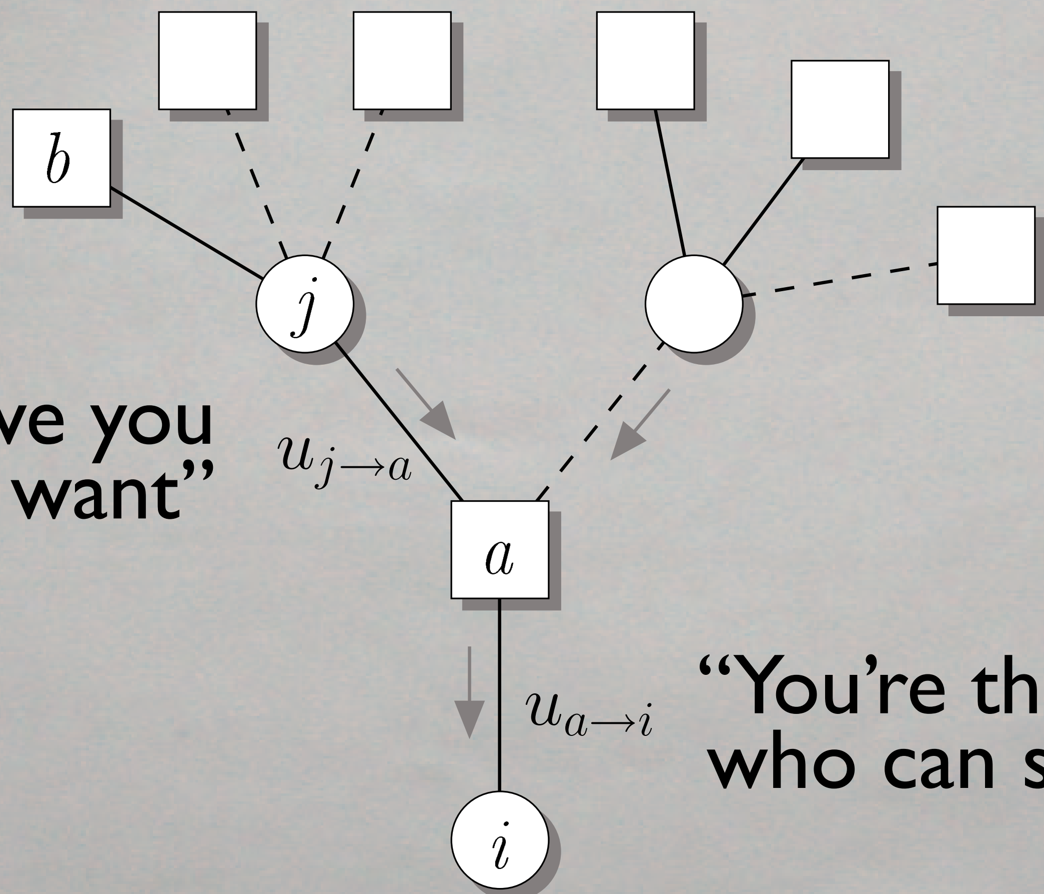
- An idea from statistical physics: there is another transition, from a unified "cloud" of solutions to separate clusters.
- Is this why algorithms fail at $\alpha \sim 2^k/k$?



The Physicists' Algorithm

- A "message-passing" algorithm:

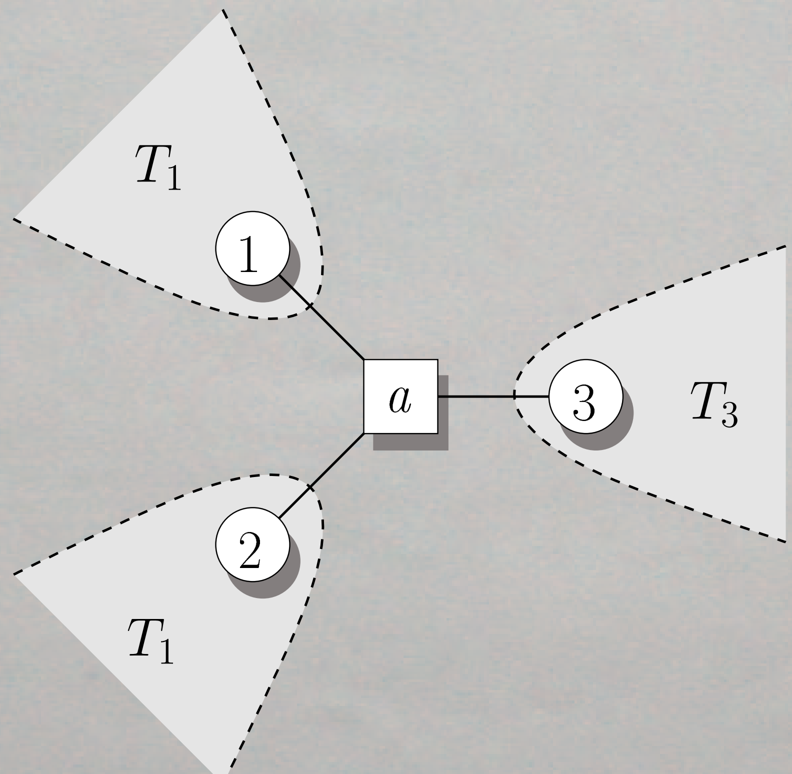
"I can't give you what you want"



"You're the only one who can satisfy me"

Why Does It Work?

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



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

Shameless Plug

This book rocks! You somehow manage to combine the fun of a popular book with the intellectual heft of a textbook.

— Scott Aaronson

A treasure trove of information on algorithms and complexity, presented in the most delightful way.

— Vijay Vazirani

A creative, insightful, and accessible introduction to the theory of computing, written with a keen eye toward the frontiers of the field and a vivid enthusiasm for the subject matter.

— Jon Kleinberg

Oxford University Press, 2011

THE NATURE *of* COMPUTATION

Cristopher Moore
Stephan Mertens