

# Phase Transitions in Satisfiability and Coloring

*Rigorously Proved Results*

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# The satisfiability problem (SAT)

- Boolean variables  $x_1, x_2, \dots, x_n$ .
- Literals: Boolean variables or negations of them.
- Clause: Disjunction of literals ( $x_1 \wedge x_2 \wedge \neg x_3$ ).
- Formula: Conjunction of clauses (Conjunctive Normal Form – CNF).

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- Formula: Conjunction of clauses (Conjunctive Normal Form – CNF).
- Satisfying truth assignment: One that has at least one true literal in every clause.
- Satisfiability Problem (SAT): Given a formula  $\phi$ , is it satisfiable?
- $k$ -SAT: Every clause contains exactly  $k$  literals.

# The DPLL procedure for SAT

- At every step, set a literal to either “true” or “false.”
- Clauses where a “true” occurrence appears are deleted.
- “False” occurrences of literals are deleted from all clauses they occur.
- If the current formula is empty, return “yes”; if it contains an empty clause, return “no”.

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- **Unit clause Rule:** Always set “true” clauses with a single literal.
- **Splitting Rule:** if no unit clauses exist, first try setting to true a suitably selected literal. In case of failure, backtrack and try setting it to false.

# The $k$ -colorability problem ( $k$ -COL)

- Given a graph  $G = (V, E)$  decide whether its vertices can be colored with at most  $k$  colors so that no adjacent vertices get the same color.

# The List Coloring algorithm

Input: A graph  $G$  together with a list of possible  $k$  colors for each of its vertices.

- At every step, choose a color from a list and assign it to its vertex.
- Delete this vertex and also delete the selected color from neighboring vertices.
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- If the graph becomes empty, return “yes”; if a vertex with an empty list appears, return “no”.
- Vertices with one element in their list are given priority.
- If one color from a list fails, backtrack and try the others.

# Average complexity

- Having an “appropriate” distribution (model of randomness) is crucial: there are results stating that SAT is “easy” on average, but they assume ad hoc distributions of the instances.
- Example of a distribution that gives rise to easy instances of SAT: Each literal gets into each clause independently with probability  $p$  (the length of a clause is a random variable).
- We will consider random instances of  $k$ -SAT, for fixed  $k$ .

# Two models for random $k$ -SAT

- $G_{n,p}$ : Each clause is independently selected with probability  $p$  to be included in the formula (the number of clauses, i.e. the length of the formula, is a random variable).
- $G_{n,m}$ : Exactly  $m$  clauses are uniformly, independently and with replacement selected to be included in the formula.

# Density

*Density* (ratio of number of clauses to number of variables ratio):

- In  $G_{n,m}$  :  $r = \frac{m}{n}$ .

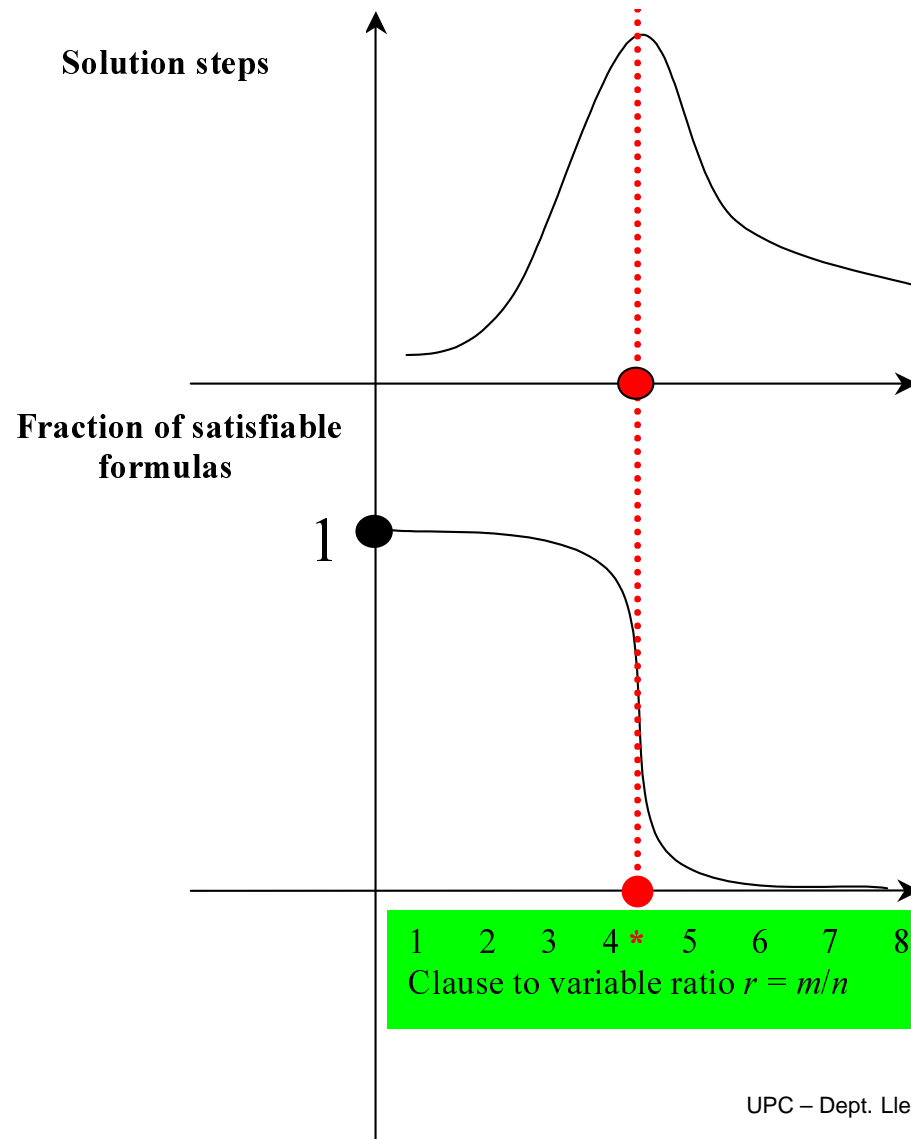
- In  $G_{n,p}$  :  $r = \frac{8p\binom{n}{3}}{n}$ .

Density is assumed to be constant.

If  $p = \frac{3r}{4n^2}$ , then in  $G_{n,p}$  expected length (number of clauses) of a formula is  $rn$ .

# Phase transition — experiments

[Mitchell et al. 1992] and other groups:



# Phase transition II

General experimental observation: for each fixed  $k$  (amenable to experimentation), there is a constant  $r_k^*$  such that:

- If  $r$  is “away” from  $r_k^*$ , then the number of DPLL calls is small, while if  $r$  is close to  $r_k^*$ , it is large.
- If  $r < r_k^*$ , then the formula is a.s. satisfiable, while if  $r > r_k^*$  the formula is a.s. unsatisfiable (“a.s.” means with probability approaching 1 asymptotically with the number of variables).

Analytic (but non-rigorous) verification of the later “decision” threshold (cavity and replica symmetry breaking methods of Statistical Physics) in papers by Mertens, Mézard, Parisi, and Zecchina.

# Phase transition III

For  $k = 3$  experiments and analytic heuristics suggest that  $r_3^* \simeq 4.2$ .

Also, it has been rigorously settled that for 2-SAT:  $r_2^* = 1$  [de la Vega, Goerdt, Chvátal & Reed].

**Open problem for 3-SAT:** (i) Formally prove the existence of  $r_3^*$  and (ii) formally compute its value.

# Friedgut's theorem

**Theorem Friedgut '97** *There is a sequence  $r^*(n)$  such that  $\forall \epsilon :$*

- $\Pr[\phi_{r^*(n)-\epsilon} \text{ is SAT}] \rightarrow 1.$
- $\Pr[\phi_{r^*(n)+\epsilon} \text{ is SAT}] \rightarrow 0.$

In other words, the transition interval can be made arbitrarily thin (sharp transition).

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- **Still open question:** Does  $r^*(n)$  converge? If yes, to what value?

**Corollary** *If  $\Pr[\phi \text{ is SAT}] > \epsilon$  finally for all  $n$ , then*  
 $\Pr[\phi \text{ is SAT}] \rightarrow 1.$

# Upper bounds for 3-SAT

- First: 5.19 (circa 1983) – observed by several researchers independently – *Markov's inequality*
- Current best: 4.506 Dubois, Boukhad, & Mandler (1999) – *typical formulas*
- Several *rigorous* (as opposed to experimental) intermediate results between 1983 and 1999.

# The basic upper bound technique

Let  $\phi$  be a random formula and  $S(\phi)$  the random class of its satisfying truth assignments (s.t.a.). Then

$$\Pr[\phi \text{ is satisfiable}] = \Pr[|S(\phi)| \geq 1] \leq \mathbb{E}(|S(\phi)|).$$

Since  $\mathbb{E}(|S(\phi)|) = (2(\frac{7}{8})^r)^n$  we obtain  $r^* < 5.19$ .

But why experiments suggest  $r^* \simeq 4.2$ ?

*Rare* formulas with *many* s.t.a. contribute *too much* to the expectation  $\mathbb{E}(|S(\phi)|)$  (**Lottery paradox**).

# How to improve the upper bound

Thin  $S(\phi)$  (the set of all satisfying truth assignments) so that the “unrealistic” expectation of the cardinality of  $S(\phi)$ , due to the Lottery paradox, gets smaller.

Examine not the whole space of possible formulas, but a subset of it such that the formulas of the subset are:

- *typical* and
- less prone to “unrealistic” expectation of the number of satisfying truth assignments (Dubois et al.).

# Algorithms for lower bounds

- Let  $r_l$  denote the lower bound for  $r^*$  that we try to compute.
- Consider DPLL with a suitable heuristic for choosing a literal in the splitting step.
- Prove that for  $r < r_l$ , the heuristic a.s. succeeds.
- Analyze DPLL without backtracking (i.e. if failure is reported before an application of the splitting rule, this failure is considered permanent).
- The more sophisticated a heuristic is, the more difficult or impossible it's probabilistic analysis is.

# Algorithmic lower bounds for 3-SAT

- First: 2.99 Chao and Franco (1986). They introduced many basic analysis techniques
- Current best: 3.52 Kaporis, Kirousis and Lalas (2001).
- Progress in the case of lower bounds is much slower and the techniques more involved (compared with upper bounds).
- Also, there is strong experimental evidence that the algorithmic approach cannot overcome a barrier around 3.9, which is considerably below the putative threshold value (4.25). Why?

# The Y2K problem

By the first moment method it is easy to show the the putative threshold for  $k$ -SAT is at most  $(\ln 2)2^k$ .

An easy algorithmic bound [Chvátal and Reed, 1992] shows the the threshold is  $\Omega((1/k)2^k)$  (as  $k$  grows large).

Many attempts to algorithmically close the gap from below failed. Why?

PS The term Y2K refers to the question “Why  $2^k$ ?” The term was coined in September 1999 during a workshop in Trieste on NP-completeness and phase transitions.

# The geometry of truth assignments

Consider the space of all truth assignments with the Hamming distance. Then:

- For densities below certain value, all satisfying truth assignments form a unique cluster.
- As the density increases, the clusters break down into exponentially many.
- Moreover, exponentially many clusters correspond to a local minimum (with respect to the number of unsatisfiable clauses).

# The geometry of assignments cont'ed

- As a consequence, local search algorithms are not expected to produce results beyond the breaking down of the unique cluster.
- Hard satisfiability region (densities below but close to the threshold).

Results by Biroli and Monasson; Mézard, Parisi and Zecchina and others, e.g. recently by Mézard, Palassini, and Rivoire.

Recent rigorous results: Achlioptas and Ricci-Tersenghi; Mézard, Mora, and Zecchina (2005).

# Survey Propagation

- An algorithm for  $k$ -SAT (for small values of  $k$ ) that behaves very nicely up to the threshold.
- Difficult, or perhaps impossible, to rigorously analyze Survey Propagation.
- Inspired from the Statistical Mechanics approach to phase transition phenomena like SAT (reminiscent of Belief Propagation).

Seminal exposition paper: Mézard, Parisi, and Zecchina, Science, 2002.

# What is the way out?

**Conclusion:** Non-algorithmic approaches for lower bounds should be tried.

# The second moment method

Let  $X$  be a non-negative variable (usually a *counting* variable) that depends on  $n$ .

- Lottery Paradox: As  $n$  grows large  $\mathbb{E}(X)$  may also grow large, but yet  $\Pr[X > 0]$  may approach zero.
- However if  $\mathbb{E}(X^2)$  (the *second moment*, essentially the *variance*) does not approach infinity too fast compared to  $\mathbb{E}(X)$ , then it may turn that  $\Pr[X > 0]$  stays away from zero. Formally:

$$\Pr[X > 0] \geq \frac{(\mathbb{E}(X))^2}{\mathbb{E}(X^2)}.$$

First used for  $k$ -SAT by Achlioptas and Moore, 2002.

# The solution of the Y2K problem

- Try the Second Moment Method, by defining  $X$  to be the number of satisfying truth assignments of a random instance of  $k$ -SAT.
- Unfortunately the method does not work, because  $X$  has a large second moment.
- Achlioptas and Moore, 2002: Count in  $X$  the satisfying truth assignments that in each clause falsify at least one literal (in addition to satisfying one). This symmetry requirement reduces the variance.
- They showed that  $(\ln 2/2)2^k - O(1)$  is a lower bound to the threshold.
- Achlioptas and Peres, 2003 improved the above to  $(\ln 2)2^k - O(k)$ .

# What about $k$ -COL?

- Łuczak, 1991: The chromatic number of almost all  $G_{n,p=d/n}$  graphs, with a given fixed average degree  $2d$ , may take only two consecutive integer values.
- Unfortunately, until very recently, not much was known about the value of these integers.
- Achlioptas and Naor (2004). Let  $k_d$  be the smallest integer  $k$  such that  $d < k \ln k$ . Almost all  $G_{n,d/n}$  random graphs have chromatic number either  $k_d$  or  $k_d + 1$ .

# $k$ -COL continued

- Method of Proof: Second moment where  $X$  counts the number of balanced  $k$ -colorings of  $G_{n,d/n}$ .
- Difficulty: The second moment of  $X$  turns out to be a sum of exponential terms. Locating the term with the largest base, which essentially gives the value of the sum, proved out to be a difficult task.

# Random regular graphs?

Progress is much slower.

- Achlioptas and Moore (2004): The chromatic number of random regular graphs with  $n$  vertices and degree  $2d$  ( $d$  fixed) may take only the values  $k_d, k_d + 1, k_d + 2$ , where  $k_d$  is again the smallest integer  $k$  such that  $d < k \ln k$ .
- Shi and Wormald (2004): Algorithmic analogous results for values of  $d$  up to 10.
- Also, almost all 4-regular graphs have chromatic number 3, and
- almost all 6-regular graphs have chromatic number 4.

# 5-regular graphs?

- Replica Symmetry Breaking – Survey Propagation (Krzakala, Pagnani, Weigt, 2004): almost all 5-regular graphs have chromatic number 3.
- Also, the solution space of 3-colorings of 5-regular graphs has many clusters. Therefore, algorithmic techniques are expected to be hard.
- Until recently, the only rigorous result for 5-regular graphs is that almost all of them have chromatic number 3 or 4.
- Second Moment: Fails when  $X$  counts 3-colorings, even if they are balanced. Not enough symmetry, so the second moment (variance) is large.

# Stable 3-colorings

Colorings where each vertex has neighbors of both the other two legal colors.

Balanced: each color is assigned to an equal number of vertices.

Díaz, Grammatikopoulos, Kaporis, Kirousis, Pérez and Sotiropoulos (2005): 5-regular graphs are 3-colorable with positive probability.

Method of proof: Apply second moment to the number of stable, balanced 3-colorings on 5-regular graphs.

Result: A 5-regular graph is 3-colorable with positive probability independent of its size.

# “Off the press”

Kemkes and Wormald: Padded up this probability to 1 (asymptotically).

Technique: Using the previous result that:

$$\Pr[X > 0] \geq \frac{(\mathbb{E}(X))^2}{\mathbb{E}(X^2)} \sim \text{constant.}$$

They showed that:

$$\Pr_Y[X > 0] \geq \frac{(\mathbb{E}_Y(X))^2}{\mathbb{E}_Y(X^2)} \sim 1,$$

by conditioning over the number of the cycles of the subgraph that “work against colorability”.