Percolation and Phase Transition in SAT

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Abstract. Erdös and Rényi proved in 1960 that a drastic change occurs in a large random graph when the number of edges is half the number of nodes: a giant connected component surges. This was the origin of percolation theory, where statistic mechanics and mean field techniques are applied to study the behavior of graphs and other structures when we remove edges randomly.
In the 90's the study of random SAT instances started. It was proved that in large 2-SAT random instances also a drastic change occurs when the number of clauses is equal to the number of variables: the formula almost surely changes from satisfiable to unsatisfiable. The same effect, but at distinct clause/variable ratios, was detected in k-SAT and other random models.
In this paper we study the relation between both phenomena, and establish a condition that allows us to easily find the phase transition threshold in several models of 2-SAT formulas. In particular, we prove the existence of a phase transition threshold in scale-free random 2-SAT formulas.

1 Introduction

Percolation theory describes the behavior of connected components in a graph when we remove edges randomly. Erdös and Rényi [10] are considered the initiators of this theory. In this seminal paper on graph theory they proposed a random graph model $G(n,m)$ where all graphs with n nodes and m edges are selected with the same probability. Gilbert [14] proposed a similar model $G(n,p)$ where n is also the number of nodes, and every $\binom{n}{2}$ possible edge is selected with probability p. For not very sparse graphs (when $p\,n^2 \to \infty$), both models have basically the same properties taking $m = \binom{n}{2}p$. Erdös and Rényi [11] also studied the connectivity on these graphs and proved that

- when $n\,p < 1$, i.e. $m < n/2$, a random graph almost surely has no connected component larger than $\mathcal{O}(\log n)$,
- when $n\,p = 1$, i.e. $m = n/2$ a largest component of size $n^{2/3}$ almost surely emerges, and
- when $n\,p > 1$, i.e. $m > n/2$, the graph almost surely contains a unique giant component with a fraction of the nodes and no other component contains more than $\mathcal{O}(\log n)$ nodes.

Phase transitions is a phenomenon that has been observed and studied in many AI problems. Many problems have an order parameter that separates a region of solvable and unsolvable problems, and it has been observed that hard problems occur at critical values of this parameter. Mitchell et al. [15] found this phenomena in 3-SAT when the ratio between number of clauses and variables is $m/n \approx 4.3$. Gent and Walsh [13] observed the same phenomenon with clauses of mixed length. Chvátal and Reed [8] proved that, in 2-SAT, a random formula with $(1+o(1))\,c\,n$ clauses of size 2 over n variables, is satisfiable with probability $1 - o(1)$, when $c < 1$, and unsatisfiable with probability $1 - o(1)$, when $c > 1$, where $o(1)$ represents a quantity tending to zero as n tends to infinity.

There is a close relationship between SAT problems and graphs. Both, percolation on graphs and phase transition in SAT (or other AI problems) are critical phenomena and both can be studied using mean field techniques from statistical mechanics. Percolation theory has been used and inspired works in the literature about random SAT and satisfiability threshold, e.g. in Achlioptas et al. [1] to determine the satisfiability threshold of 1-in-k SAT and NAE 3-SAT formulas. Some results on graphs have been previously extended to 2-SAT. For instance, Sinclair and Vilenchik [18] adapted Achlioptas processes for graphs into formulas. Bollobás et al. [6] investigated the scaling window of the 2-SAT phase transition, finding the critical exponent of the order parameter and proving that the transition is continuous, adapting results of Bollobás [5] for Erdös-Rényi graphs. The relationship between percolation in random graphs and phase transition in random 2-SAT formulas is suggested in many other works. For instance, Monasson et al. [17] when study the phase transition in $2+P$-SAT (a mixture of $(1-p)m$ clauses of size 2 and $p\,m$ clauses of size 3) already mention that *"It is likely that the 2SAT transition results from percolation of these loops..."*. However, to the best of our knowledge, this is the first time that percolation theory has been used to establish a general criterion for the existence of phase transitions in 2-SAT formulas.

Given a random 2-SAT formula with m clauses over n variables, we can construct an Erdös-Rényi graph where the $2\,n$ literals are nodes, and the m clauses are edges. In the percolation point $m = (2\,n)/2$ of this graph a *giant component* emerges. Just at the same point $m = n$ it is located the 2-SAT phase transition threshold. However, despite the coincidence in the point, the relation between both facts is not direct: a giant component in the graph is not the same as a giant (hence, unsatisfiable) loop of implications in the SAT formula. The connection between two edges $a \leftrightarrow b$ and $b \leftrightarrow c$ in the graph is given by a common node (literal) b. Whereas, in the SAT formula, the resolution between $a \vee b$ and $\neg b \vee c$ is throughout a variable b that is affirmed in one clause and negated in the other. In this paper, we elaborate on the relation of giant components in graphs and unsatisfiability proofs in 2-SAT formulas.

This paper proceeds as follows. In Section 3 we will define a criterion for the existence of a giant loop in the implication graph. Since this giant loop will contain almost surely a variable and its negation, this will imply the unsatisfiability of the original formula. However, in some cases, the unsatisfiability comes from the existence of a small unsatisfiable core of clauses in the formula. In other words, the existence of giant components implies the unsatisfiability of the formula, but the inverse implication is false. In Section 2, we study 1-SAT as an example of formulas where all minimal unsatisfiable cores are small. In Section 4, we use the criterion to prove the existence of a phase transition in (classical) random 2-SAT formulas, a result originally proved by Chvátal and Reed [8]. Recently, Friedrich et al. [12] have found a lower bound for a possible phase transition in scale-free random 2-SAT formulas [3], when $\beta < 1/2$. In Section 5 we prove the existence of an upper bound (which implies the existence of the SAT-UNSAT phase transition) and extend the result for $\beta > 1/2$. Finally, in Section 6, we discuss again the effect of small unsatisfiable cores in phase transitions.

2 Phase Transition in 1-SAT

In most models of random formulas, as the number of variables tend to infinite, existence of small minimal unsatisfiability cores of clauses (*cores* for short) become much less probable than existence of large cores. Therefore, in such cases, the percolation and phase transition thresholds coincide. However, there are other models where the unsatisfiability of the formula is due to the existence of small cores. In this second case, there is not a proper phase transition threshold. In order to analyze this second phenomena, we will study the phase transition in 1-SAT formulas.

1-SAT formulas are conjunctions of one-literal clauses. The only possible minimally unsatisfiability core is $\{a, \neg a\}$, for some variable a. Therefore, in this model all cores are small. There are satisfiable 1-SAT formulas of any size (since we can have repeated clauses). However, a random formula with just one repeated variable has probability 1/2 to be unsatisfiable. In order to find the phase transition threshold, if it really exists, we may compute the probability of a formula with m clauses over n variables to not contain repeated variables:

$$P(n,m) = \frac{n-1}{n}\,\frac{n-2}{n}\cdots\frac{n-m+1}{n} = \frac{(n-1)!}{(n-m)!\,n^{m-1}}$$

Using Stirling's approximation and $\lim_{n\to\infty}(1-1/n)^n = e^{-1}$, for big values of $n-m$, this probability can be approximated[1] as:

$$\begin{aligned} P(n,m) &\sim \frac{\sqrt{2\pi(n-1)}\left(\frac{n-1}{e}\right)^{n-1}}{\sqrt{2\pi(n-m)}\left(\frac{n-m}{e}\right)^{n-m} n^{m-1}} \\ &= e^{1-m}\,(1-1/n)^{n-1/2}\,(1-m/n)^{m-n-1/2} \\ &\sim e^{-m}\,(1-m/n)^{m-n-1/2} = \frac{1}{\sqrt{1-m/n}}\left(\frac{1}{e^{m/n}\,(1-m/n)^{1-m/n}}\right)^n \end{aligned}$$

[1] As usual, we write "$f(n) \sim g(n)$, for big values of n", if $g(n)$ and $f(n)$ are asymptotic, i.e. $\lim_{n\to\infty} f(n)/g(n) = 1$.

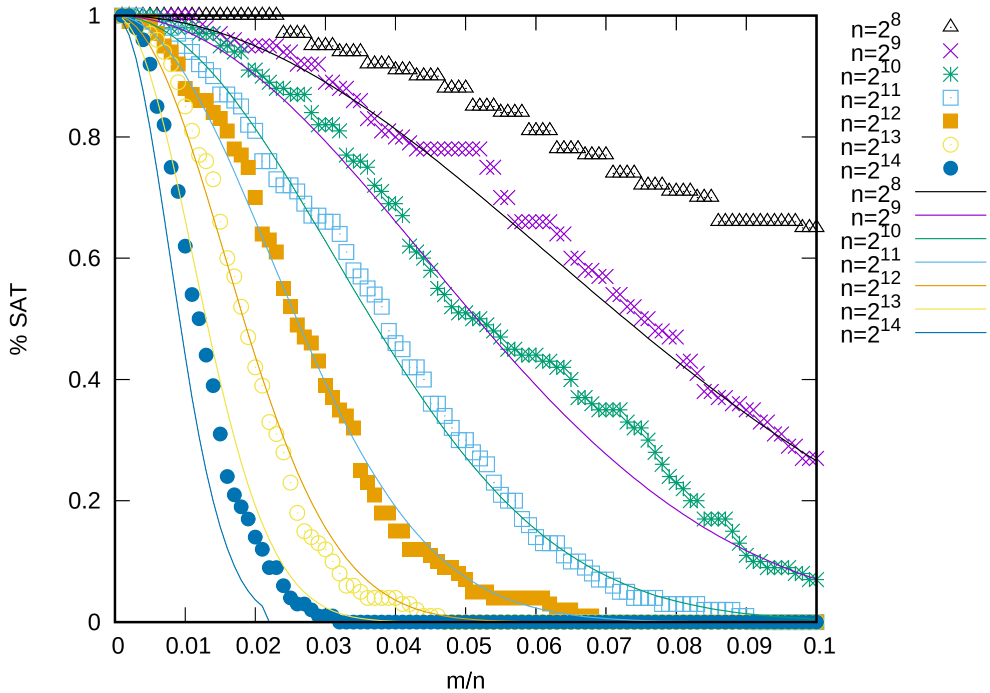

Fig. 1. Fraction of satisfiable random 1-SAT formulas as a function of clause/variable for n between 2^8 and 2^{14}. Dots represent experimental data, and continuous lines the prediction $P(n,m) = \frac{1}{\sqrt{1-m/n}} \left(\frac{1}{e^{m/n}\,(1-m/n)^{1-m/n}}\right)^n$ for the probability of not repeated variables. The experimental fraction is approximated repeating the experiment for 50 formulas.

If we replace $m = c\,n$, with $c < 1$, we get

$$P(n,cn) \sim \frac{1}{\sqrt{1-c}} \left(\frac{1}{e^c\,(1-c)^{1-c}}\right)^n$$

When $n \to \infty$, the function $P(n,cn)$ has a phase transition, but it is located at the critical value of c solving: $e^c\,(1-c)^{1-c} = 1$. However, the unique solution of this equation is $c = 0$.

Therefore, 1-SAT has a phase transition point, when $m = c\,n$ and $n \to \infty$, but it is located at $c = 0$. In Figure 1 we represent the fraction of satisfiable formulas with respect to m/n found experimentally and the theoretical prediction for the occurrence of the fist repeated variable. Since the repetition of variables does not imply the unsatisfiability of the formula, the experimental data are moved to the right of theoretical data.

In Section 5, we will see another example of formulas with a phase transition at $c = 0$, and where cores are small. We conjecture that, in a random SAT model, when small cores are more probable than large cores, the phase transition threshold is $c = 0$. And, when large cores are more probable than small cores, then the percolation threshold, obtained with our criterion, and the phase transition threshold are equal.

3 A Criterion for Phase Transition in 2-SAT

In the following we will consider 2-SAT formulas defined as multisets of (possibly repeated) clauses $x \vee y$, where a clause is a pair of literals. A literal is a variable x or its negation $\neg x$. We identify $\neg\neg x$ with x, and we assume that clauses do not contain repeated variables.

Unsatisfiability proofs of 2-SAT formulas are characterized by *bicycles*. We define a *cycle* in a 2-SAT formula F as a sequence of literals $x_1, \dots, x_n$ such that, $\neg x_i \vee x_{i+1}$, for any $i = 1, \dots, n-1$, and $\neg x_n \vee x_1$ are clauses[2] of F. We define a *bicycle* in a 2-SAT formula as a cycle $x_1, \dots, x_n$ such that there exists a variable a satisfying $\{a, \neg a\} \subseteq \{x_1, \dots, x_n\}$.

A 2-SAT formula is unsatisfiable if, and only if, it contains a bicycle [4,8].

We will also consider random graphs with n nodes and m edges,[3] and connected components, defined as subsets of nodes such that any pair of them is connected by a path inside the component. A random graph of size n is said to contain a *giant connected component* if almost surely[4] it contains a connected component with a positive fraction of the nodes. Given a model of random graphs, we say that c is the percolation threshold if any random graph with n nodes and more than $c\,n$ edges almost surely contains a giant component. In a random graph, the degree of a node x, noted k_x, is a random variable. The random variable k represents the degree of a random node chosen with uniform probability.[5]

As we commented in the introduction, we can represent any 2-SAT formula as a graph where nodes are literals, and clauses $a \vee b$ are edges between literals a and b. However, a connected component in the graph is not necessarily an unsatisfiability proof of the formula.

First, in a random SAT formula, we may have repeated clauses, which means that from m clauses we will obtain less than m edges. However, in the limit

[2] In some papers, bicycles are defined in terms of implications, where a clause $x \vee y$ is represented as a pair of implications $\neg x \rightarrow y$ and $\neg y \rightarrow x$. In the percolation processes we remove randomly selected edges. Therefore, in order to avoid the possibility of removing an implication $\neg x \rightarrow y$ and preserve the associated $\neg y \rightarrow x$ in the percolation process, we only deal with clauses, and not implications.

[3] We will deal with distinct models of random graphs where every graph has a distinct probability of being chosen.

[4] *Almost surely* means that, in the model of random graph, as $n \rightarrow \infty$, the probability tends to one.

[5] In some of the models of random graphs that we will consider, not all degrees of nodes follow the same probability distribution. Therefore, we will distinguish between k and k_x.

$n \to \infty$, with a linear number of clauses $m = \mathcal{O}(n)$, and a quadratic number of possible clauses, the number of repeated clauses is negligible. In classical 2-SAT random formulas, since literals are chosen independently with uniform probability, the generated graph will be an Erdös-Rényi graph following the model $G(2\,n, m)$.

Second, graph connected components and cycles are not the same structure. Therefore, the existence of a giant connected component and the existence of a giant cycle are independent facts.

Theorem 1 establishes a criterion for the existence of a giant bicycle in a formula. The proof of the theorem resembles Molloy-Reed criterion [16,9] for the existence of a giant component in a graph when $\frac{E[k^2]}{E[k]} > 2$, where k is the degree of a random node, and E denotes expectation. However, notice that, in Theorem 1, the 2 of Molloy-Reeds criterion is replaced by a 3.

Interestingly, this criterion depends not only on the expected degree of nodes, but also on the expected square degree of the nodes, hence on the variability of node's degrees. The variability on the nodes degree plays an important role in the location of the percolation threshold. For instance, in the Erdös-Rényi model, the percolation threshold is located at $m/n = 1/2$, hence the expected degree of nodes is $1/2$. However, the expected degree of nodes belonging to the same connected component[6] of size r is, at least, $(r-1)/r \approx 1$. This discrepancy is only possible if the variability in node's degree is high. This also explains why, in regular random formulas, where we impose variables to occur exactly the same number of times (instead of the same average number of times), we get distinct phase transition thresholds.

Theorem 1. *Let F be a random 2-SAT formula generated with a model where (1) the number of occurrences of literals x and $\neg x$, noted k_x and $k_{\neg x}$, follow the same and independent probability distribution*[7] *and (2) the probability of clause $x \vee y$ only depends on the probability distributions for k_x and k_y. Then, F contains a giant bicycle if, and only if,*

$$\frac{E[k^2]}{E[k]} + E[k] > 3$$

Or, equivalently:

$$\frac{E[K^2]}{E[K]} > 3$$

where $K_x = k_x + k_{\neg x}$, for every variable x.

Proof. In percolation theory we get a giant connected component when a node i, connected to a node j, is also connected in average to at least one other node.

[6] Recall that minimally connected components are trees, where the number of edges is equal to the number of nodes minus one.

[7] The distribution is the same for k_x and $k_{\neg x}$, but it can be different for the number of occurrences of distinct variables k_x and k_y.

Formally, when the expected degree of i, conditioned to the fact that i and j are connected, is $E[k_i \mid i \leftrightarrow j] = 2$.

In our case, in order to emerge a giant cycle, when there is a clause $x \vee y$, we have to find another clause containing $\neg x$. It is difficult to find a criterion expressing such condition dealing with literals. Instead, we will reason about variables. When we have a clause containing variable x, i.e. $x \vee y$ or $\neg x \vee y$, for some literal y, we have to find another clause that contains $\neg x$, or x, respectively, allowing us to continue the construction of the cycle. In this situation, the expected number of other clauses containing x is 2, that added to the original clause gives the 3. Let $\pm x \vee y$ express the fact "$x \vee y \in F$ or $\neg x \vee y \in F$, for some literal y, and let $K_x = k_x + k_{\neg x}$ be the number of occurrences of variable x. Formally, our criterion can be written as

$$E[K_x \mid \pm x \vee y] > 3$$

This criterion is the necessary and sufficient condition to continue the construction of a set of clauses, ensuring that the probability that this set contains a fraction of the literals tends to one.

Using Bayes, we have

$$\begin{aligned} E[K_x \mid \pm x \vee y] &= \sum_{k=0}^{\infty} k\, P(K_x = k \mid \pm x \vee y) \\ &= \sum_{k=0}^{\infty} k\, \frac{P(K_x = k \wedge \pm x \vee y)}{P(\pm x \vee y)} \\ &= \sum_{k=0}^{\infty} k\, \frac{P(\pm x \vee y \mid K_x = k) P(K_x = k)}{P(\pm x \vee y)} \end{aligned}$$

Under the conditions of the theorem we have that the probability of a clause conditioned to the fact that the number of occurrences of one of its variables is k is $P(\pm x \vee y \mid K_x = k) = \frac{k}{n-1}$ and, the probability of any clause is $P(\pm x \vee y) = \frac{E[K_x]}{n-1}$. Therefore

$$\begin{aligned} E[K_x \mid \pm x \vee y] &= \sum_{k=0}^{\infty} k\, \frac{\frac{k}{n-1} P(K_x = k)}{\frac{E[K_x]}{n-1}} \\ &= \frac{\sum_{k=0}^{\infty} k^2\, P(K_x = k)}{E[K_x]} = \frac{E[K_x^2]}{E[K_x]} \end{aligned}$$

Now, since $K_x = k_x + k_{\neg x}$ and k_x and k_x follow the same distribution, we have $E[K_x] = 2\, E[k_x]$ and $E[K_x^2] = 2\, E[k_x^2] + 2\, E^2[k_x]$. Therefore,

$$\frac{E[K^2]}{E[K]} = \frac{E[k^2]}{E[k]} + E[k]$$

Finally, we prove that any giant cycle in a formula is, with high probability, a bicycle. I.e. any set of literals containing a fraction of all literals will almost surely contain also a literal a and its negation $\neg a$. We are in the presence of $2n$ literals and a giant cycle of size $c\,n$ (where $0 < c < 1$). The probability of having two given literals in the giant cycle is roughly c^2. But then, the giant cycle can have any of the n pairs of the form $(x, \neg x)$ with probability $1-(1-c^2)^n$, which tends exponentially fast to 1. $\square$

The previous theorem ensures that, when $\frac{E[K^2]}{E[K]} > 3$, there is a giant bicycle containing a fraction of the literals, and the formula is unsatisfiable. However, if the formula is unsatisfiable, it can be due to a *small* bicycle, and we can not conclude $\frac{E[K^2]}{E[K]} > 3$. In other words, Theorem 1 establish a sufficient (but not necessary) condition for unsatisfiability of random 2-SAT formulas, which result into an upper bound for the phase transition point. However, we conjecture that, either giant bicycles are more probable than small bicycles and the percolation threshold (obtained with the criterion) is equal to the phase transition point, or, if small bicycles are more probable, the phase transition point is at $c = 0$.

An interesting question is what is the size of the greatest cycle at the (exact) percolation threshold $\frac{E[K^2]}{E[K]} = 3$ of 2-SAT formulas. In the case of graphs, the greatest connected component at the percolation threshold $\frac{E[k^2]}{E[k]} = 2$ has size $\mathcal{O}(n^{2/3})$. Therefore, it does not contain a fraction of the nodes as in the case $\frac{E[k^2]}{E[k]} > 2$. In the case of formulas, we would probably find a similar situation. However, the analysis would require more sophisticated tools.

4 Classical 2-SAT Formulas

Theorem 1 may be used to find the phase transition point in terms of number of clauses divided by number of variables. In this section, we apply the technique to (classical) random 2-SAT formulas.

We start with a formula (or graph), not necessarily in the critical threshold. Then, we apply a percolation process where a fraction $1-p$ of randomly selected clauses (edges) are removed, such that the remaining p fraction of edges are in the critical threshold. If we start with the complete formula with all possible $2^2\binom{n}{2}$ clauses over n variables, and remove clauses with uniform probability, this process generates a (classical) random 2-SAT formula in the SAT-UNSAT transition point.

If k'_x is the number of occurrences of literal x in the original graph, then, after removing the $(1-p)$ fraction, the new distribution on the number of occurrences is $P(k_x) = \sum_{k'_x=k_x}^{\infty} P(k'_x)\binom{k'_x}{k}\,p^k\,(1-p)^{k'_x-k}$. Using this binomial distribution we get the moments $E[k_x] = p\,E[k'_x]$ and $E[k_x^2] = p^2\,E[(k'_x)^2] + p(1-p)E[k'_x]$. If we impose the criterion to this new formula we get

$$\frac{p^2\,E[(k')^2] + p(1-p)E[k']}{p\,E[k']} + p\,E[k'] = 3$$

Hence

$$p = \frac{2}{\frac{E[(k')^2]}{E[k']} + E[k'] - 1}$$

For the complete formula we have $k'_x = 2(n-1)$ for any literal, therefore $p = 1/(2n - 5/2)$. The expected number of clauses in the phase transition threshold is

$$E[m] = 2^2 \binom{n}{2} p = \frac{2n(n-1)}{2n-5/2} = n + \mathcal{O}(1)$$

This proves that the clause/variable fraction at the 2-SAT phase transition threshold is at most $m/n = 1$, reproducing the results of Chvátal and Reed [8].

For the expected moments we get $E[k] = 1$ and $E[k^2] = 2$, for number of occurrences of literals, and $E[K] = 2$ and $E[K^2] = 6$, for number of occurrences of variables.

Now, we want to apply the same technique to regular random 2-SAT formulas. These are random formulas where the number of occurrences of a literal minus the number of occurrences of another literal is, at most, one. In this case, the conditions of Theorem 1 are not fulfilled: k_x and $k_{\neg x}$ are not independent random variables. Since in a random regular formula $k_x = k_{\neg x}$, if this formula contains a clause $x \vee y$, we only need to require that $E[K_x \mid x \vee y] = 2$ in order to ensure that there is another clause containing $\neg x$, allowing us to continue the construction on the bicycle. With this new criterion, and reproducing the proof of Theorem 1, we obtain that the criterion for the existence of a giant bicycle in a regular random formula is

$$\frac{E[K^2]}{E[K]} = 2$$

In the case of classical regular random formulas, all literals have the same number of occurrences $k_x = m/n$, hence $E[K] = 2m/n$ and $E[K^2] = (2m/n)^2$. Applying the criterion to the formula, without any need of percolation process, we get $\frac{E[K^2]}{E[K]} = \frac{(2m/n)^2}{2m/n} = 2$. Therefore, $m/n = 1$ is an upper bound for the phase transition point, reproducing the results of Boufkhad et al. [7].

5 Scale-free 2-SAT Formulas

Random scale-free formulas were introduced by Ansótegui et al. [3]. They are formulas where the number of occurrences of a randomly chosen variable follows a power-law distribution. The same distribution has been observed in most industrial SAT instances used in the SAT competitions [2]. These formulas are the result of encoding real-world problems into SAT. Therefore, it has been conjectured that such model is more accurate to reproduce the properties of industrial instances, that are the target of modern SAT solvers.

Random scale-free formulas are parametric on an exponent $\beta \in [0, 1]$. Clauses are chosen independently, with possible repetitions, like in the classical random model. However, the probability to be chosen is not uniform, and depends on the probability of their literals:

$$P(x_1 \vee \ldots \vee x_n) \sim \prod_{i=1}^{n} P(x_i)$$

being zero when the clause contains repeated variables. The probability of a literal and its negation is the same $P(x) = P(\neg x)$, and the probability of variable x_i is:

$$P(x_i) \sim i^{-\beta}$$

Ansótegui et al. [3] proved that in this model, the number of occurrences K of a random variable follows a power-law distribution $P(K) \sim K^{-\delta}$ where $\delta = 1 + 1/\beta$.

Recently, Friedrich et al. [12] have proved that scale-free random 2-SAT formulas with exponent $\delta > 3$ and clause/variable ratio $m/n < \frac{(\delta-1)(\delta-3)}{(\delta-2)^2}$ are satisfiable with probability $1 - o(1)$.[8] This gives a lower bound for a possible phase transition point, in terms of δ. They conjecture that this bound is tight and that this phase transition exists. Replacing $\delta = 1 + 1/\beta$ (according to [3]) in [12], we get:

Scale-free random 2-SAT formulas with exponent $\beta < 1/2$ and clause/variable ratio $m/n < \frac{1-2\beta}{(1-\beta)^2}$ are satisfiable with probability $1 - o(1)$.

In the first statement of the following theorem, we prove that when the clause/variable ratio exceeds this value, formulas are almost surely unsatisfiable.

Theorem 2. *Scale-free random 2-SAT formulas with exponent* $\beta < 1/2$ *and clause/variable ratio* $m/n > \frac{1-2\beta}{(1-\beta)^2}$ *are unsatisfiable with probability* $1 - o(1)$.
Scale-free random 2-SAT formulas over n *variables, exponent* $1/2 < \beta < 1$*, and*

$$m > \frac{2\beta - 1}{(1-\beta)^2} n^{2(1-\beta)} + \mathcal{O}(1)$$

clauses, are unsatisfiable with probability $1 - o(1)$.

Proof. In the case of scale-free formulas we cannot start the percolation process from the complete formula, since the uniform-random deletion of clauses do not give rise to scale-free formulas. We have to start with an already scale-free formula, over the phase threshold. The process of percolation in this case preserves the scale-free structure. Therefore, we can simply impose the criterion to the original formula. We will do all the computations using the number of occurrences of variables K_x, instead of the number of occurrences of the literal k_x. Since the election of every variable of every clause is independent (we can

[8] In their paper, they write β instead of δ, but we prefer to use β with the same meaning as in [3].

neglect repetitions of variables in clauses in the limit), the number of occurrences of $x = 1, \dots, n$ follows a binomial distribution

$$P(K_x = K) = \binom{2m}{K}\left(\frac{x^{-\beta}}{\sum_{i=1}^n i^{-\beta}}\right)^K\left(1 - \frac{x^{-\beta}}{\sum_{i=1}^n i^{-\beta}}\right)^{2m-K}$$

In the limit $m \to \infty$ the distribution approaches a Poisson distribution where

$$\begin{aligned}
E[K_x] &= \frac{x^{-\beta}}{\sum_{i=1}^n i^{-\beta}}\,2m \\
E[K_x^2] &= \left(\frac{x^{-\beta}}{\sum_{i=1}^n i^{-\beta}}\,2m\right)^2 + \frac{x^{-\beta}}{\sum_{i=1}^n i^{-\beta}}\,2m
\end{aligned}$$

Recall that in scale-free formulas K_x follows a distinct probability distribution for every variable x, therefore we have to average over all variables

$$\begin{aligned}
E[K] &= 1/n \sum_{x=1}^n E[K_x] = 1/n \sum_{x=1}^n \frac{x^{-\beta}}{\sum_{i=1}^n i^{-\beta}}\,2m = \frac{2m}{n} \\
E[K^2] &= 1/n \sum_{x=1}^n E[K_x^2] \\
&= 1/n \sum_{x=1}^n \left(\frac{x^{-\beta}}{\sum_{i=1}^n i^{-\beta}}\,2m\right)^2 + \frac{x^{-\beta}}{\sum_{i=1}^n i^{-\beta}}\,2m \\
&= \frac{4m^2}{n}\,\frac{\int_1^n x^{-2\beta}\mathrm{d}x}{\left(\int_1^n i^{-\beta}\mathrm{d}i\right)^2} + \frac{2m}{n} \\
&= \frac{4m^2}{n}\,\frac{(1-\beta)^2}{1-2\beta}\,\frac{n^{1-2\beta}-1}{(n^{1-\beta}-1)^2} + \frac{2m}{n}
\end{aligned}$$

Where we approximate sums as integrals (which is correct in the limit), and we assume that $\beta \neq 1, 1/2$.

Imposing the criterion we get

$$\frac{E[K^2]}{E[K]} = 2m\frac{(1-\beta)^2}{1-2\beta}\,\frac{n^{1-2\beta}-1}{(n^{1-\beta}-1)^2} + 1 = 3$$

Hence

$$m = \frac{1-2\beta}{(1-\beta)^2}\,\frac{(n^{1-\beta}-1)^2}{n^{1-2\beta}-1}$$

$$m = \begin{cases}
\dfrac{1-2\beta}{(1-\beta)^2}n + \mathcal{O}(1) & \text{if } \beta < 1/2 \\[2ex]
\dfrac{2\beta-1}{(1-\beta)^2}n^{2(1-\beta)} + \mathcal{O}(1) & \text{if } 1/2 < \beta < 1 \\[2ex]
\dfrac{2\beta-1}{(1-\beta)^2} & \text{if } 1 < \beta
\end{cases}$$

□

From [3,12] and Theorem 2 we can conclude:

Corollary 1. *Scale-free 2-SAT formulas over n variables and exponent $\beta < 1/2$ have a SAT-UNSAT phase transition threshold when the variable/clauses ratio is*

$$m/n = \frac{1-2\beta}{(1-\beta)^2}$$

We have experimentally analyzed the fraction of satisfiable random scale-free 2-SAT formulas depending on the parameter β and fraction of clause/variable m/n. The results are plotted in Figure 2, for formulas with $n = 10^5$ variables. We observe that the phase transition predicted by Theorem 2 is quite precise, except when $\beta \gtrsim 1/2$. In the limit $n \to \infty$, the fraction of satisfiable formulas with n variables and $c\,m$ clauses tends to zero when $c > 0$. However, as the number of clauses needed to make the formula unsatisfiable grows as $n^{2(1-\beta)}$, when β is close to 1/2 the confluence is very slow.

In order to test experimentally the second statement of the lemma, we have analyzed the fraction of satisfiable formulas when m is around $m = c\,n^{2(1-\beta)}$, where $c = \frac{2\beta-1}{(1-\beta)^2}$. In fact, we have analyzed the fraction of satisfiable formulas with respect to $m/n^{2(1-\beta)}$. In figure 3, we show the results for $\beta = 3/4$ and for $m/n^{2(1-\beta)}$ between 0 and $2\,c$. We observe that, for distinct values of n, the transition between SAT and UNSAT is around $m/n^{2(1-\beta)} \approx c$. However, for increasing values of n the transition does not seem to become more abrupt.

6 Unsatisfiability by Small Cores

In the proof of Theorem 2 we have already seen that, when $\beta > 1/2$ the number of clauses needed to make the formula unsatisfiable is sub-linear. Therefore, the phase transition factor –understood as a constant c such that, on the limit $n \to \infty$, formulas with less that $c\,n$ clauses are satisfiable and those with more than $c\,n$ clauses are unsatisfiable– is zero. In this section, we will prove that, when β exceeds a certain bound, scale-free formulas become unsatisfiable due to a small subset of clauses containing variables with small indexes. Moreover, this result holds for clauses of any size.

Theorem 3. *A random scale-free formula over n variables, exponent β and $\mathcal{O}(n^{(1-\beta)k})$ clauses of size k is unsatisfiable with probability $1 - o(1)$.*

Proof. Recall that the probability of a variable to be selected in the construction of a clause is $P(x_i) \sim i^{-\beta}$. This means that the probability of a clause only containing the smallest k variables is

$$\begin{aligned} P(x_1 \vee \ldots \vee x_k) &\geq P(x_1) \cdots P(x_k)\,(1/2)^k \\ &= \frac{1^{-\beta} \cdots k^{-\beta}}{\left(\sum_{i=1}^{n} i^{-\beta}\right)^k}\,(1/2)^k \end{aligned}$$

This inequality would be an equality, if we allow tautologies and simplifiable clauses (i.e. repeated variables) in formulas.

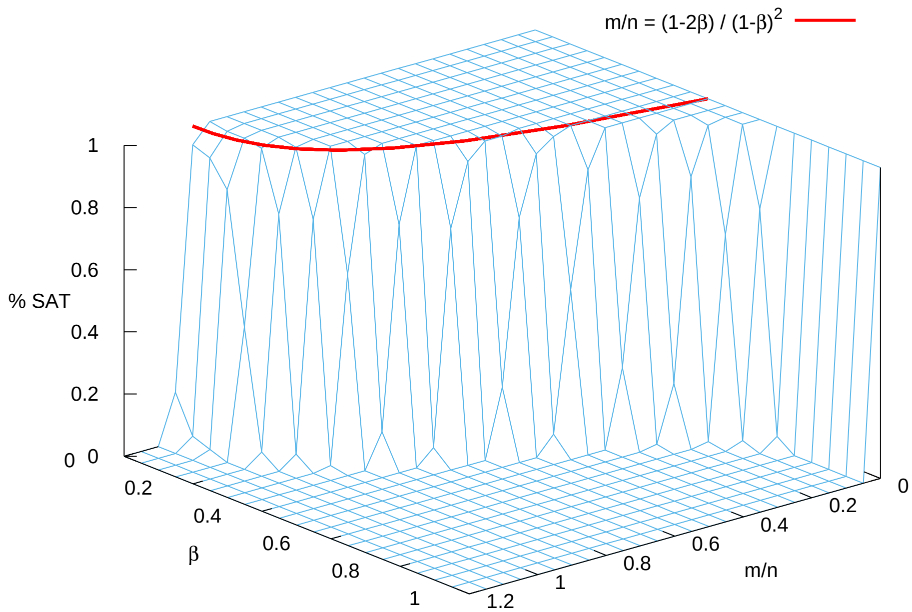

Fig. 2. Fraction of satisfiable formulas as a function of parameter β and fraction of clause/variables m/n. The number of variables is $n = 10^5$ and the fraction is approximated repeating the experiment for 10 formulas at every point. We also draw the theoretical threshold $m/n = \frac{1-2\beta}{(1-\beta)^2}$.

Using the continuous approximation we get

$$\begin{aligned} P(x_1 \vee \ldots \vee x_k) &\geq \frac{1^{-\beta} \cdots k^{-\beta}}{\left(2 \sum_{i=1}^{n} i^{-\beta}\right)^k} \approx \frac{(k!)^{-\beta}}{\left(2 \int_1^n i^{-\beta}\, \mathrm{d}i\right)^k} \\ &= (k!)^{-\beta} \left(\frac{1-\beta}{2(n^{1-\beta}-1)}\right)^k \end{aligned}$$

when $\beta \neq 1$.

All other clauses with variables $1, \ldots, k$ and distinct signs have the same probability. In the limit $n \to \infty$, when the number of clauses is $\mathcal{O}(n^{(1-\beta)k})$, the formula will contain all 2^k clauses of the form $\pm x_1 \vee \ldots \vee \pm x_k$ with probability $1 - o(1)$. □

As in classical random formulas, the expected number of truth assignments that satisfy a scale-free random formula is $2^n(1-2^{-k})^m$. This imposes a linear upper bound on the number of clauses of satisfiable scale-free formulas, i.e. a random scale-free formula with $m = c\,n$ clauses of size k over n variables such that $c > 2^k \log 2$ is unsatisfiable with probability $1 - o(1)$. Therefore, the bound

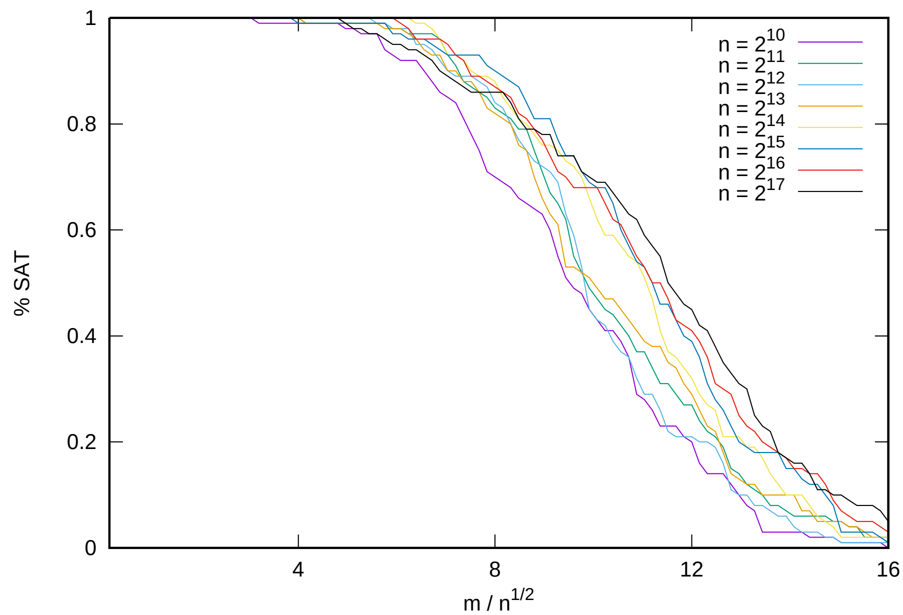

Fig. 3. Fraction of satisfiable formulas as a function of $m/n^{2(1-\beta)} = m/\sqrt{n}$, for $\beta = 3/4$, and distinct values of n between 2^{10} and 2^{17}. Notice that for $\beta = 3/4$ the constant is $c = \frac{2\beta-1}{(1-\beta)^2} = 8$. Every point is computed repeating the experiment for 100 formulas.

in Theorem 3 only *improves* this other linear bound when $(1-\beta)k < 1$, hence when $\beta > 1 - 1/k$.

Theorem 3 predicts that the number of clauses in a satisfiable scale-free 2-SAT formula cannot grow faster that $\mathcal{O}(n^{2(1-\beta)})$, due to the emergence of small cores. When $1/2 < \beta < 1$, second statement of Theorem 2, predicts exactly the same exponent $2(1-\beta)$ for the emergence of a giant bicycle. This suggest that, in this range of β, the probability of existence of a small and a giant unsatisfiable core of clauses is similar. However, experimental results (see Figure 3) suggest that the SAT-UNSAT transition is quite smooth, like in classical 1-SAT. This suggest that small cores are, in fact, more prominent. Another argument in this direction is as follows:

Let $C(V)$ be the subset of clauses only containing variables of the subset V of variables. The greater $|C(V)|/|V|$ is, the higher is the probability to have an unsatisfiable core inside $C(V)$. In the case of scale-free random k-SAT formulas, let C_r be the set of clauses only containing variables $\{1, \ldots, r\}$. We can estimate

$$E\left[\frac{|C_r|}{r}\right] = \frac{m}{r}\left(\frac{\sum_{i=1}^{r} i^{-\beta}}{\sum_{i=1}^{n} i^{-\beta}}\right)^k \approx \frac{m}{r}\left(\frac{r^{1-\beta}-1}{n^{1-\beta}-1}\right)^k$$

For $(1-\beta)k \geq 1$, i.e. $\beta < 1 - 1/k$, the maximum of this function is $r = \infty$. For $(1-\beta)k < 1$, i.e. $\beta > 1 - 1/k$, the maximum is finite:

$$r = (1-(1-\beta)k)^{-1/(1-\beta)}$$

Notice that $(1-\beta)k$ is the exponent predicted by Theorem 3, and that for 2-SAT, $1 - 1/k = 1/2$. Therefore, we get another proof that at $\beta = 1 - 1/k$ we get a change in the behavior of scale-free random k-SAT formulas. When $n \to \infty$, for $\beta \leq 1-1/k$ the most probable is to get a very large core that involves a fraction of the whole set of clauses. For $\beta > 1-1/k$ the most probable is to get a small core only involving a finite set of clauses and variables $\{1, \ldots, (1-(1-\beta)k)^{-1/(1-\beta)}\}$.

7 Conclusions

In this paper we have shown that percolation-based or, in general, mean field techniques are a useful tools for the analysis of phase transition in SAT. We have applied these techniques to prove the existence of a phase transition threshold in random 2-SAT formulas, reproducing some results of Chvátal and Reed [8].

We have also applied the percolation-based technique to prove the existence of a phase transition threshold in random scale-free 2-SAT formulas. In this case, we find an unsatisfiability result (upper bound) that, together with Friedrich et al.'s [12] satisfiability result (lower bound), proves the existence of the threshold.

Finally, we conjecture and argue that, when in a model the existence of small unsatisfiable cores in formulas is more probable than the existence of large cores, the SAT-UNSAT transition is smoother and the clause/variable threshold tends to zero.

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