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Phase Transitions and Satisfiability Threshold[†]

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Summary by Vincent Puyhaubert

Abstract

The 3-SAT problem consists in determining if a boolean formula with 3 literals per clause is satisfiable. When the ratio between the number of clauses and the number of variables increases, a threshold phenomenon is observed: the probability of satisfiability appears to decrease sharply from 1 to 0 in the neighbourghood of a fixed threshold value, conjectured to be close to 4.25. Although a threshold value has been provably obtained for the similar problem 2-SAT and for closely related problems like 3-XORSAT, there is still no proof for the 3-SAT problem.

Recent works have so far provided only upper and lower bounds for the potential location of the threshold. We present here a survey of methods giving upper bounds. We also introduce generating functions as a new generic tool and rederive some of the most significant upper bounds in a simple uniform manner.

1. Introduction

We consider boolean formulæ over a set of variable $x_1, \ldots, x_n$ (where the x_j range over $\{0, 1\}$ or $\{\text{true}, \text{false}\}$). A literal is either a variable x_j or a negated variable $\neg x_j$. It is known that each boolean formula admits a conjunctive normal form, being a conjunction of clauses, themselves disjunctions of literals. A 3-SAT formula is then such a formula with exactly 3 literals per clause. A typical formula is then for example:

$$\Phi = (x_1 \vee \neg x_2 \vee x_4) \wedge (\neg x_2 \vee \neg x_3 \vee x_5) \wedge (x_1 \vee \neg x_4 \vee \neg x_5) \wedge (x_3 \vee \neg x_4 \vee \neg x_5).$$

We will choose the model where each clause is composed of a set of three literals from distinct variables. There are then $8\binom{n}{3}$ distinct clauses and $8^m\binom{n}{3}^m$ formulæ with m clauses. Other models may be occasionally used for convenience in calculations, for example, the three literals may be ordered and not necessarily distinct so that there would be $8n^3$ clauses. All these models are easily proved to be equivalent with respect to the probability of satisfiability.

In Figure 1, a *phase transition phenomenon* can be observed regarding the satisfiability of these formulæ when they are drawn at random. As the ratio r of the number m of clauses to the number n of variables increases, the probability of satisfiability drops abruptly from nearly 1 to nearly 0.

From these experiments, it is believed that there exists a critical value r_3 such that for any $\epsilon > 0$, the probability of satisfiability tends to 1 for $r < r_3 - \epsilon$ (as m and n tend to infinity), and tends to 0 for $r > r_3 + \epsilon$. Experiments suggest for r_3 the value 4.25 ± 0.05. However, so far, only successive

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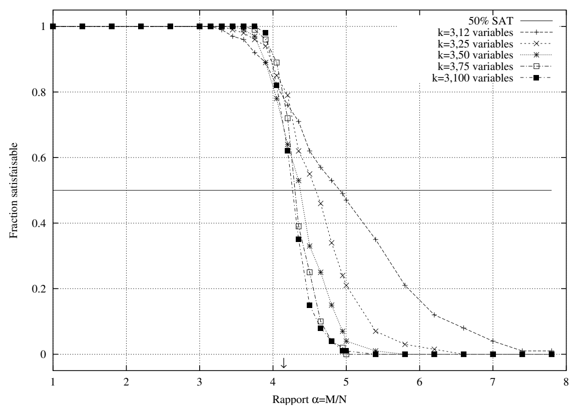

FIGURE 1. Ratio of satisfiable formulæ with respect to the parameter m/n.

upper and lower bounds of the potential location of the threshold have been obtained. The table below lists the bounds successively established for the 3-SAT threshold. The bounds marked with a star admit an extension to k-SAT for any k.

Lower bounds for 3-SAT threshold		Upper bounds for 3-SAT threshold	
2.9*	Chao and Franco (1986,1990) [4]	5.191*	Franco and Paull (1983) [8]
2/3*	Chvátal and Reed (1992)	5.081	El Mafthoui and Fernandez de la Vega (1993) [6]
1.63	Broder et al. (1993) [3]	4.762*	Kamath et al. (1995) [12]
3.003*	Frieze and Suen (1996) [10]	4.643*	Dubois and Boufkhad (1997) [5]
3.145	Achlioptas (2000) [1]	4.602	Kirousis et al. (1998) [13]
		4.596	Janson et al. (1999) [11]
		4.506	Dubois et al.

Apart from these works, Friedgut [9] also proved that there exists a sequence (γ_n) such that for any $\epsilon > 0$, the probability of satisfiability tends to 1 as m and n increase under the constraint $m/n < \gamma_n - \epsilon$, while it tends to 0 under the constraint $m/n > \gamma_n + \epsilon$. But it is not known whether the sequence (γ_n) converges. The limiting value γ would be the threshold r_3.

The aim of the present paper is to present some of the most significant upper bounds on the satisfiability threshold. We will specially focus on enumerative proofs, with the help of generating functions. For lower bounds, one can refer to the surveys by Franco [7] and Achlioptas [2].

2. **Expectations of the Number of Solutions**

The first bound for 3-SAT threshold has been obtained by several authors as a direct application of the first-moment method to the random variable giving the number of solutions of a random formula. Under an enumerative perspective, it can be seen as a direct application of the following simple remark: *Each positive integer k satisfies $k \geq 1$.* From there, one has the following inequality:

$$\big|\Phi \text{ satisfiable}\big| \leq \big|(\Phi, S) \text{ such that } \Phi \text{ is satisfied by } S\big|. \qquad (1)$$

Let S be an assignment of the n variables to values in $\{0,1\}$ and $C = \pm x_i \vee \pm x_j \vee \pm x_k$ a clause. There is only one way to choose the signs of the three literals in order to have the value of C be false under S: each literal must have the opposite sign of its assignment. Then, there are 7 ways to choose the signs in order to render C true. The number of clauses satisfied by any given S is then $7\binom{n}{3}$. Since S is a solution of a 3-SAT formula Φ if and only if all clauses of Φ are satisfied by S, for any assignment, there are exactly $7^m\binom{n}{3}^m$ formulas with m clauses which admit S as a solution.

The cardinality of the pairs (Φ, S) such that S is a solution of Φ is then given by $2^n 7^m \binom{n}{3}^m$. Dividing each term of (1) by the total number of formulæ $8^m\binom{n}{3}^m$ gives (with $r = m/n$):

$$\mathbf{P}(\Phi \text{ satisfiable}) \leq \left(2\left(\frac{7}{8}\right)^r\right)^n. \tag{2}$$

Hence, for $r > \ln(2)/\ln(8/7) \approx 5.191$, the right-hand side of (2) tends to 0 as n tends to infinity, and so does the probability of satisfiability. This gives the first upper bound obtained by Franco and Paull.

3. Prime Implicants

In the previous section, we have bounded the number of satisfiable formulæ by their number of solutions. Since a formula may have from 1 to almost 2^n solutions, the upper bound provided may be very coarse. The next idea is to group some of the solutions which look very close to each other and enumerate only these groups for each formula. In this way, it may be possible to get an improved upper bound on the satisfiability threshold.

This leads to the definition of partial assignments and prime implicants. A partial assignment A is simply an assignment of a subset of the n variables (possibly all, so that solutions are also partial assignments). Let us say that A satisfies a formula Φ if and only if all complete assignments A' extending A are solutions of Φ. A necessary and sufficient condition for this is that in each clause of Φ, there exists at least one of the three literals which is true under A. If there are k missing variables in a partial assignment A, then A "groups" 2^k solutions together.

A natural order may be placed on partial assignments. We say that A is smaller than B if we can remove some assigned variables from B to get A. A prime implicant is then a partial assignment which satisfies Φ and is *minimal* with respect to this order. Any satisfiable formula has then at least one prime implicant since it has at least one solution and the set of partial assignments is then non-empty. As in the previous section, we get from there the inequality (see (1)):

$$|\Phi \text{ satisfiable}| \leq |(\Phi, I) \text{ such that } I \text{ is a prime implicant of } \Phi|. \tag{3}$$

Note that the sets of solutions grouped together by two distinct partial assignments are not necessarily disjoint. Some formulæ may have more prime implicants than solutions. But in fact, the expectation of the number of prime implicants of a random formula appears to be smaller by an exponential factor.

Let I be a partial assignment of k variables. Then, all clauses in a formula Φ that admits I as a prime implicant must contain at least one literal satisfied by I. Let $A_{n,k}$ be the set of such clauses and $\alpha_{n,k}$ their number (it is clear that this quantity depends only on k and n and does not depend on the names or values of the variables assigned in I).

Let then Φ be a formula which admits I as a prime implicant. Recall that I has to be minimal with respect to the order defined earlier. Let I' be obtained from I by removing a variable x_i from the set of assigned variables. Then I' can not satisfy Φ, which means that at least one clause in Φ must be rendered false by I'.

Hence, at least one clause is of the form $\pm x_i \vee a \vee b$ where the sign of the literal x_i makes this literal positive under I and where a and b are literals from unassigned variables or false under I. Let C_{x_i} be the set of such clauses. Then all these sets have the same number of elements $\beta_{n,k}$ and are mutually disjoint. In order to build a formula for which I is a prime implicant, we need to choose m clauses among $A_{n,k}$ so that in k subsets, we must pick at least one element. The number of such formulæ is then the number $I_{n,k,m}$ whose generating function is given by

$$I_{n,k}(z) = \sum_{m\geq 0} I_{n,k,m} \frac{z^m}{m!} = e^{z(\alpha_{n,k}-k\beta_{n,k})} \left(e^{z\beta_{n,k}} - 1\right)^k .$$

Finally, since there are $\binom{n}{k}2^k$ partial assignments of k variables, the total number of pairs (Φ, I) such that I is a prime implicant for Φ is given by:

$$\big|(\Phi, I)\big| = \sum_{k=0}^{n} \binom{n}{k} 2^k m!\, [z^m]\, e^{z(\alpha_{n,k}-k\beta_{n,k})} \left(e^{z\beta_{n,k}} - 1\right)^k . \tag{4}$$

The next step depends on the following general remark: if (f_k) is a sequence of positive reals and $f(z) = \sum f_k z^k$ then for all $s > 0$ within the domain of convergence of $f(z)$:

$$f_k \leq \frac{f_0}{s^k} + \cdots + f_k + f_{k+1}s + \cdots = \frac{f(s)}{s^k} \quad \text{and thus} \quad f_k \leq \min_s \frac{f(s)}{s^k}.$$

From now on, we set $k = \alpha n$, $m = rn$ and make use of the upper bounds $\alpha_{n,k} - k\beta_{n,k} \leq \frac{1}{3}k^2(3n-k)$ and $\beta_{n,k} \leq \frac{1}{2}(2n-k)^2$. From (3) and (4) one determines:

$$\mathbf{P}(\Phi \text{ satisfiable}) \leq \sum_{\alpha\in\{0,1/n,\ldots,1\}} f(\alpha)^n \tag{5}$$

with

$$f(\alpha) = \left(\tfrac{3r}{4e}\right)^r \frac{2^\alpha}{\alpha^\alpha(1-\alpha)^{1-\alpha}} e^{\frac{u_\alpha}{3}\alpha^2(3-\alpha)} \left(e^{\frac{u_\alpha}{2}(2-\alpha)^2} - 1\right)^\alpha {u_\alpha}^{-r}$$

where u_α makes $f(\alpha)$ minimal. For $r > 4.89$, one verifies that the maximum of f is strictly under 1. The probability of satisfiability in then bounded from above by $(n+1)\delta^n$ with $\delta < 1$ and thus, tends to 0 as n tends to infinity. The idea of prime implicant was first introduced by Olivier Dubois and an improvement of this idea led to the value 4.762 obtained by Kamath.

4. Negatively Prime Solutions

The next idea is to introduce a partial order on the set of solutions. Define B to be an assignment smaller than A if we can change the values of some of its variables from 0 to 1 to get A. We now propose to enumerate only pairs (Φ, S) where S is a maximal solution with respect to this order. In fact, it is very difficult to find for any given assignment a simple characterization of formulæ for which it is a maximal solution; consequently we have to deal with a weaker definition of *local maximal solution* (also called *negatively prime solution* or NPS). This is a solution for which changing the value of any variable from 0 to 1 no longer gives a solution of our formula. This amounts to considering solutions which do not admit a greater solution that differs in exactly one variable. Once more, we start from the inequality:

$$|\Phi \text{ satisfiable}| \leq |(\Phi, S) \text{ such that } S \text{ is a NPS of } \Phi| . \tag{6}$$

Let A be an assignment giving the value 0 to k variables and Φ a formula for which A is an NPS. Then, all clauses of Φ must belong to the set A_n of all $7\binom{n}{3}$ clauses satisfied by A (as seen in Section 2). Now, if any variable x_i assigned to 0 is changed to 1, there must be at least one clause in Φ that is no longer satisfied by this new assignment: at least one clause must be of the form $\neg x_i \vee a \vee b$ where a and b are false under A. If we denote by C_{x_i} this set of clauses (for each variable assigned to 0), then all these sets have the same number $\binom{n-1}{2}$ of elements and are mutually disjoint. As in the previous section, since there are $\binom{n}{k}$ solutions with k variables assigned to 0, we get:

$$\left|(\Phi, A \text{ NPS})\right| = \sum_{k=0}^{n} \binom{n}{k} m!\,[z^m]\, e^{z\left(7\binom{n}{3}-k\binom{n-1}{2}\right)} \left(e^{z\binom{n-1}{2}}-1\right)^k.$$

By $[z^m]\, f(z)+g(z) = [z^m]\, f(z) + [z^m]\, g(z)$, this gives a closed-form expression:

$$\left|(\Phi, A \text{ NPS})\right| = m!\,[z^m]\, e^{z4\binom{n}{3}} \left(2e^{z\binom{n-1}{2}}-1\right)^n. \tag{7}$$

The same remark as in the previous section, Stirling formula, and the change of variable $z = \delta\binom{n-1}{2}$ provide that for any $\delta > 0$ with $m = rn$:

$$\mathbf{P}(\Phi \text{ satisfiable}) \le \left(\left(\frac{3r}{8e}\right)^r \frac{e^{\frac{4}{3}\delta}\left(2e^{\delta}-1\right)}{\delta^r}\right)^n. \tag{8}$$

This expression is minimized by $\delta\left(\frac{4}{3}+\frac{2e^\delta}{2e^\delta-1}\right) = r$ and, with such a δ, is strictly smaller than 1 as soon as $r > 4.643$. Hence, the probability of satisfiability tends to 0 for every r greater than this value. This bound was first obtained by Dubois and can be extended to k-SAT for any k. It is so far the best *general* upper bound known for k-SAT.

5. Typical Formulæ

In the previous section, we have enumerated all pairs of formulæ and NPS. However, there may be a negligible proportion of formulæ with a huge number of such solutions. In this case, when we enumerate the NPS for these formulæ, the contribution to the whole sum may be non negligible. The idea here is to throw away some formulæ and then, enumerate the NPS only for the retained formulæ, which are called *typical* formulæ. The whole calculation will not be given here, only the idea that led to the proof.

In this section, we introduce for convenience a variation of the model used so far (this does not affect the threshold value). A formula consists in a sequence of $3m$ literals among the $2n$ possible ones, where 3 consecutive literals form a clause (thus literals within clauses are allowed to repeat). Let $\omega_{p,l}$ be the random variable giving the fraction of variables which appear in the formula p times where l of the occurrences are positive. Then, when $m = rn$, the variable quantity $\omega_{p,l}$ follows a Poisson limit law in the following sense: let $\kappa_{p,l} = \frac{1}{2^l}\binom{p}{l}\frac{\lambda^k}{k!}e^{-\lambda}$ with $\lambda = 3r$, then

$$\forall l, p \quad \forall \epsilon > 0 \qquad \mathbf{P}\left(|\omega_{l,p} - \kappa_{l,p}| > \epsilon\right) \underset{n\to\infty}{\longrightarrow} 0. \tag{9}$$

Let $x_{\max}$ be an integer and $\epsilon > 0$. A formula will be called typical if and only if

$$\forall 0 \le p \le l \le x_{\max} \qquad \left|\omega_{l,p}(\Phi) - \kappa_{l,p}\right| \le \epsilon.$$

For any fixed $x_{\max}$ and ϵ, as a consequence of (9), the set of non typical formulæ is negligible. Hence:

$$\mathbf{P}(\Phi \text{ satisfiable}) \le \frac{\left|(\Phi \text{ typical}, S \text{ NPS})\right|}{|\Phi|} + o(1). \tag{10}$$

With $x_{max} = 56$ and $\epsilon = 10^{-15}$, for $r = 4.506$, the expectation of the number of NPS among typical formulæ was proven to be $o(1)$. This value, obtained by Dubois, is the best currently known upper bound for the 3-SAT threshold.

Remark. In fact, one last refinement is needed in order to achieve the upper bound 4.506. In a formula, if one switches all variables appearing more often under positive form than under negative form, in the sense that all positive occurrences (resp. all negative) are replaced by the negated literal (resp. the positive), the satisfiability of the formula remains unchanged, as does the number of solutions. However, the number of NPS is lowered. The last idea in the proof, is to enumerate, for typical formulæ, not their own number of NPS but the one of their so called *totally unbalanced* form.

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