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A Better Upper Bound for the Unsatisfiability Threshold

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Abstract. Let ϕ be a random Boolean formula that is an instance of 3-SAT. We consider the problem of computing the least real number κ such that if the ratio of the number of clauses over the number of variables of ϕ strictly exceeds κ, then ϕ is almost certainly unsatisfiable. By a well known and more or less straightforward argument, it can be shown that $\kappa \leq 5.191$. This upper bound was improved by Kamath, Motwani, Palem, and Spirakis to 4.758, by first providing new improved bounds for the occupancy problem. There is strong experimental evidence that the value of κ is around 4.2. In this work, we show that this upper bound can be improved to 4.667. Our proof is elementary and short, and does not use unverifiable mechanical calculations. Moreover it generalizes in a straightforward manner to k-SAT, for $k > 3$.

1. Introduction

Let ϕ be a random 3-SAT formula on n Boolean variables $x_1, \ldots, x_n$. Let m be the number of clauses of ϕ. The clauses-to-variables ratio of ϕ is defined to be the number m/n. We denote this ratio by r. The problem we consider in this paper is to compute the least real number κ such that if r strictly exceeds κ, then the probability of ϕ being satisfiable converges to 0 as n approaches infinity. We say in this case that ϕ is asymptotically almost certainly unsatisfiable. Experimental evidence suggests that the value of κ is around 4.2. Moreover, experiments suggest that if r is strictly smaller than κ, then ϕ is asymptotically almost certainly satisfiable. Thus, experimentally, κ is not only the lower bound for unsatisfiability, but it is a threshold value where, "suddenly", probabilistically certain unsatisfiability yields to probabilistically certain satisfiability (for a review of the experimental results see [**7**]).

In the literature for this problem, the most common model for random 3-SAT formulas is the following: from the space of clauses with *exactly three* literals

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of three *distinct* variables from $x_1, \ldots, x_n$, uniformly and independently select m clauses that form the set of conjuncts of ϕ (thus a clause may be selected more than once). We adopt this model in this paper, however, the results can be generalized to any of the usual models for random formulas. The total number N of all possible clauses is $8\binom{n}{3}$, and given a truth assignment A, the probability that a random clause is satisfied by A is $7/8$. Also, given three distinct variables x_i, x_j, x_k, there is a unique clause on the variables x_i, x_j, x_k which is *not* satisfied by A. There are $\binom{n}{3}$ such clauses, and they constitute exactly the set of clauses not satisfied by A.

A proposition stating that if r exceeds a certain constant, then ϕ is asymptotically almost certainly unsatisfiable has as immediate corollary that this constant is an upper bound for κ. We use this observation in our technique to improve the upper bound for κ.

A well known "first moment" argument shows that

$$\kappa \leq \log_{8/7} 2 = 5.191.$$

To prove it, observe that the expected value of the number of truth assignments that satisfy ϕ is $2^n (7/8)^{rn}$, then let this expected value converge to zero and use Markov's inequality (this argument is expanded below). According to Chvátal and Reed [**2**], this observation is due to Franco and Paull [**4**], Simon et al. [**9**], Chvátal and Szemerédi [**3**], and possibly others.

Let $\mathcal{A}_n$ be the set of all truth assignments on the n variables $x_1, \ldots x_n$, and let $\mathcal{S}_n$ be the set of truth assignments that satisfy the random formula ϕ. The cardinality $|\mathcal{S}_n|$ is thus a random variable. Also, for an instantiation ϕ of the random formula, let $|\mathcal{S}_n(\phi)|$ denote the number of truth assignments that satisfy ϕ. (A word of caution: in order to avoid overloading the notation, we use the same symbol ϕ to denote the random formula and an instantiation of it.) We give below a rough outline of our technique.

By definition, the expected value of the number of satisfying truth assignments of a random formula, i.e., $\mathbf{E}[|\mathcal{S}_n|]$, satisfies the following relation

$$\mathbf{E}[|\mathcal{S}_n|] = \sum_{\phi} \left(\mathbf{Pr}[\phi] \cdot |\mathcal{S}_n(\phi)| \right). \tag{1.1}$$

On the other hand, the probability of a random formula being satisfiable is given by the equation:

$$\mathbf{Pr}[\text{the random formula is satisfiable}] = \sum_{\phi} \left(\mathbf{Pr}[\phi] \cdot I_\phi \right), \tag{1.2}$$

where

$$I_\phi = \begin{cases} 1 & \text{if } \phi \text{ is satisfiable,} \\ 0 & \text{otherwise.} \end{cases} \tag{1.3}$$

¿From equations (1.1) and (1.2) the following Markov's inequality follows immediately:

$$\mathbf{Pr}[\text{the random formula is satisfiable}] \leq \mathbf{E}[|\mathcal{S}_n|]. \tag{1.4}$$

It is easy to find a condiditon on κ under which $\mathbf{E}[|\mathcal{S}_n|]$ converges to zero. Such a condition, by Markov's inequality (1.4), implies that ϕ is asymptotically almost certainly unsatisfiable (this elementary technique is known as the "first moment method"). However, as in the right-hand side of equation (1.1) we may have small probabilities multiplied with large cardinalities, such a condition may be unnecessarily strong for guaranteeing only that ϕ is almost certainly unsatisfiable. In this work, instead of considering the random class $\mathcal{S}_n$ that may have a large cardinality for certain instantiations of the random formula with small probability, we consider a subset of it obtained by taking truth assignments that satisfy a local maximality condition. Thus, the condition obtained by letting the expected value of this new class converge to zero is weakened, and consequently, the upper bound for κ is lowered.

As we show in the next section, the bound for κ obtained by this sharpened first moment technique is equal to 4.667. This improves the previous best bound due to Kamath, Motwani, Palem, and Spirakis [**5**] of 4.758, which was obtained by non-elementary means. Moreover our method is not computational, i.e. it does not use any mechanical computations that do not have provable accuracy and correctness (the fact that in our method we use a computer program to find a solution of an equation with *one* unknown does not render our proof computational, because the algorithms that find solutions to such equations have provable accuracy). The bound that Kamath et al. [**5**] attain with a non-computational proof is equal to 4.87.

Notice that we can further improve our bound by selecting even smaller subsets of $\mathcal{S}_n$, by, e.g., increasing the degree of locality in selecting the maxima that represent $\mathcal{S}_n$. This is the object of current investigations to be presented elsewhere (see [**6**] for a preliminary report). Finally, our method readily generalizes to k-SAT, for $k > 3$.

2. The Results

Recall, $\mathcal{A}_n$ is the class of all truth assignments, and $\mathcal{S}_n$ is the random class of truth assignments that satisfy a random formula ϕ. We now define a class even smaller than $\mathcal{S}_n$.

DEFINITION 2.1. For a random formula ϕ, $\mathcal{S}_n^\sharp$ is defined to be the random class of truth assignments A such that (i) $A \models \phi$, and (ii) any assignment obtained from A by changing exactly one FALSE value of A to TRUE does not satisfy ϕ.

Notice that the truth assignment with all its values equal to TRUE vacuously satisfies condition (ii) of the previous definition. Consider the lexicographic ordering among truth assignments, where, as usual, the value FALSE is considered smaller than TRUE and the values of variables with higher index are of lower priority in establishing the way two assignments compare. It is not hard to see that $\mathcal{S}_n^\sharp$ is the set of elements of $\mathcal{S}_n$ that are local maxima in the lexicographing ordering of assignments, where the neighborhood of determination of local maximality is the set of assignments that differ from A in at most one position.

We now prove:

LEMMA 2.2. *The following Markov type inequality holds for* $\mathcal{S}_n^\sharp$*:*

$$\mathbf{Pr}[\text{the random formula is satisfiable}] \leq \mathbf{E}[|\mathcal{S}_n^\sharp|]. \tag{2.1}$$

PROOF. From the previous definition we easily infer that if an instantiation ϕ of the random formula is satisfiable, then $\mathcal{S}_n^\sharp(\phi) \neq \emptyset$. (Recall that $\mathcal{S}_n^\sharp(\phi)$ is the instantiation of the random class $\mathcal{S}_n^\sharp$ at the instantiation ϕ.) We also have that

$$\mathbf{Pr}[\text{the random formula is satisfiable}] = \sum_\phi \left(\mathbf{Pr}[\phi] \cdot I_\phi\right),$$

where

$$I_\phi = \begin{cases} 1 & \text{if } \phi \text{ is satisfiable,} \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

On the other hand,

$$\mathbf{E}[|\mathcal{S}_n^\sharp|] = \sum_\phi \left(\mathbf{Pr}[\phi] \cdot |\mathcal{S}_n^\sharp(\phi)|\right).$$

The lemma now immediately follows from the above. □

We also have the following:

LEMMA 2.3. *The expected value of the random variable $|\mathcal{S}_n^\sharp|$ is given by the formula*

$$\mathbf{E}[|\mathcal{S}_n^\sharp|] = (7/8)^{rn} \sum\nolimits_{A \in \mathcal{A}_n} \mathbf{Pr}[A \in \mathcal{S}_n^\sharp \mid A \in \mathcal{S}_n]. \tag{2.3}$$

PROOF. First observe that the random variable $|\mathcal{S}_n^\sharp|$ is the sum of indicator variables and then condition on $A \models \phi$ (recall, r is the number of clauses-to-number-of-variables ratio of ϕ, so $m = nr$). □

We call a change of *exactly one* FALSE value of a truth assignment A to TRUE a *single flip*. The number of possible single flips, which is of course equal to the number of FALSE values of A, is denoted by $sf(A)$. The assignment obtained by applying a single flip sf on A is denoted by A^{sf}.

We now prove that

THEOREM 2.4. *The expected value $\mathbf{E}[|\mathcal{S}_n^\sharp|]$ is at most $(7/8)^{rn}(2 - e^{-3r/7} + o(1))^n$. It follows that the unique positive solution of the equation*

$$(7/8)^r(2 - e^{-3r/7}) = 1,$$

is an upper bound for κ (this solution is less than 4.667).

PROOF. Fix a single flip sf_0 on A and assume that $A \models \phi$. Observe that the assumption that $A \models \phi$ excludes $\binom{n}{3}$ clauses from the conjuncts of ϕ, i.e., there remain $7\binom{n}{3}$ clauses to choose the conjuncts of ϕ from. Consider now the clauses that are not satisfied by A^{sf_0} and contain the flipped variable. There are $\binom{n-1}{2}$ of them. Under the assumption that $A \models \phi$, in order to have that $A^{sf_0} \not\models \phi$, it is necessary and sufficient that at least one of these $\binom{n-1}{2}$ clauses be a conjunct of ϕ. Therefore, for each of the m clause selections for ϕ, the probability of being one that guarantees that $A^{sf_0} \not\models \phi$ is $\binom{n-1}{2}/(7\binom{n}{3}) = 3/(7n)$. Therefore, the probability that $A^{sf_0} \not\models \phi$ (given that $A \models \phi$) is equal to $1 - (1 - 3/(7n))^m$. Now, there are $sf(A)$ possible flips for A. The events that ϕ is not satisfied by the assignment A^{sf} for *each* single flip sf (under the assumption that $A \models \phi$) refer to disjoint sets of clauses. Therefore, it can be easily seen that the dependencies among them are such that:

(2.4)

$$\mathbf{Pr}[A \in \mathcal{S}_n^\sharp \mid A \models \phi] \leq \left(1 - \left(1 - \frac{3}{7n}\right)^m\right)^{sf(A)} = \left(1 - e^{-3r/7} + o(1)\right)^{sf(A)}.$$

Remember, $sf(A)$ is equal to the number of FALSE values of A. Therefore, by equation (2.3) and by Newton's binomial formula, $\mathbf{E}[|\mathcal{S}_n^\sharp|]$ is bounded above by $(7/8)^{rn}(2 - (1 - 3/(7n))^{rn})^n$, which proves the first statement of the theorem.

It also follows that $\mathbf{E}[|\mathcal{S}_n^\sharp|]$ converges to zero for values of r that strictly exceed the unique positive solution of the equation $(7/8)^r(2 - e^{-3r/7}) = 1$. By Lemma 2.2, this solution is an upper bound for κ. As it can be seen by any program that computes roots of equations with accuracy of at least four decimal digits (we used Maple [**8**]), this solution is less than 4.667. □

The generalization of the previous result to the case of k-SAT, for an arbitrary $k \geq 3$ is immediate:

THEOREM 2.5. *For the case of k-SAT ($k \geq 3$), the expected value* $\mathbf{E}[|\mathcal{S}_n^\sharp|]$ *is at most* $((2^k - 1)/2^k)^{rn}(2 - e^{-kr/(2^k-1)} + o(1))^n$. *It follows that the unique positive solution of the equation*

$$\left(\frac{2^k - 1}{2^k}\right)^r (2 - e^{-kr/(2^k-1)}) = 1,$$

is an upper bound for κ *(as defined for k-SAT).*

3. Discussion

Observe that a natural extension of our technique is to consider the subclass of $\mathcal{S}_n$ which consists of the lexicographically local maxima at a fixed Hamming distance 2, or even beyond. In this case, certain dependency complications arise in the computation of the expected value of the subclass of $\mathcal{S}_n$. We have done preliminary work for the case of Hamming distance 2 (see [**6**]). It is conceivable that one might obtain interesting results by letting the degree of locality in selecting the local maxima increase unboundedly.

Finally, observe that the estimate can be probably improved further if instead of the Markov type inequality in Lemma 2.2, we use the "harmonic mean formula," of Aldous [**1**] (see our preliminary report [**6**]).

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