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Tight Thresholds for The Pure Literal Rule

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Abstract

We consider the threshold for the solvability of random k-SAT formulas (for $k \geq 3$) using the pure literal rule. We demonstrate how this threshold can be found by using differential equations to determine the appropriate limiting behavior of the pure literal rule.

1 Introduction

We consider the problem of the performance of the pure literal rule in solving a random k-CNF satisfiability problem for $k \geq 3$.

The probability space $\Omega^k_{m,n}$ is the set of all formulas in conjunctive normal form in n variables with m clauses each containing k literals. For example, the following formula is a member of $\Omega^2_{4,3}$:

$$(x_1 \vee \bar{x}_2) \wedge (x_3 \vee x_2) \wedge (x_2 \vee \bar{x}_3) \wedge (\bar{x}_1 \vee \bar{x}_3).$$

When we speak of a *random formula*, or more specifically of random k-CNF formula with m clauses and n variables, we shall mean a formula chosen uniformly at random from $\Omega^k_{m,n}$. Note that an alternative way of thinking of such a formula is that we randomly fill each of the mk "holes" with one of the $2n$ literals, each chosen independently and uniformly at random.

The *pure literal rule* is a heuristic for satisfying a CNF formula that works as follows. A *pure literal* is one whose complement does not appear in the formula (note that a literal and its complement can both be pure, in our understanding). As long as there is a pure literal available, set a pure literal to the value 1 (true), remove all clauses containing that literal, and continue. The pure literal rule is the most conservative strategy, in that it only assigns a value to a variable that will obviously maintain the satisfiability of the formula.

Threshold behavior for the pure literal rule has been studied by Broder, Frieze, and Upfal [1], who found that for sufficiently large n a random 3-CNF formula with (approximately) $1.63n$ clauses can be solved by the pure literal rule with high probability, and a random 3-CNF formula with $1.7n$ clauses is not solvable by the pure literal rule with high probability. We expand upon their work here by finding an exact threshold by considering the limiting behavior as $n \to \infty$ using differential equations. These equations can also be thought of as describing the *expected* behavior of the system for large finite values of n. (For more on this approach, see also for example [3, 4, 5, 6, 7, 8].) The question of the performance of the pure literal rule is related to the more general question of finding thresholds for the satisfiability of random k-SAT formulas; see, for example, [2].

We note that this preliminary note sketches the development of the appropriate differential equations and their solution. The justification that these differential equations accurately represent the behavior of the pure literal rule

is not fully clarified, although it is easily checked using arguments from [1] and [4] or [8], for example. A full version to be prepared in conjunction with the authors of [1] will provide more complete details.

2 The Equations

We shall think of the pure literal rule in the following manner: at each time step, if there is a pure literal available, a pure literal is chosen uniformly at random from all pure literals. That literal and its negation are then deleted (removed from consideration), and all the clauses containing the pure literal are deleted.

In the following, all the variables are scaled by a factor of n, the number of variables in the formula. This is useful in writing the appropriate differential equations. Hence (as will be seen below) if we initially have $10n$ clauses, we will represent this by a variable with value 10.

We shall describe the pure literal rule as a process running from time 0 to 1. The variables we shall use are functions of time described as follows:

- $L(t)$: the scaled number of undeleted literals remaining
- $X_i(t)$: the scaled number of undeleted literals appearing i times in the formula
- $C(t)$: the scaled number of clauses; that is, the number of clauses remaining divided by n
- $A(t)$: the average number of clauses in which a literal chosen uniformly at random from all literals appears

We may drop the explicit dependence on t when the meaning is clear.

Note that $X_0(t)$ is the scaled number of pure literals at time t. If $X_0(t) = 0$ while $C(t) > 0$, then the pure literal rule fails to find a solution; the pure literals have run out while clauses still remain. If, however, X_0 goes to 0 only as C goes to 0 (and necessarily as t goes to 1), then the pure literal rule will succeed on a random formula with high probability. Hence our goal is to determine how X_0 behaves as we vary the ratio m/n. In particular, we shall show that for some constant c_k, X_0 stays above 0 on the interval $t \in [0, 1)$ if $m/n < c_k$ and it falls below 0 for some $t < 1$ if $m/n > c_k$.

We shall now determine equations that describe the limiting behavior as $n \to \infty$ and m/n is held fixed. The initial values for C and X_i are easily determined: $C(0) = \frac{m}{n}$ and, letting $\mu = \frac{mk}{n}$, $X_i(0) = \frac{e^{-\mu}\mu^i}{i!}$, since in the limit as n goes to infinity, the distribution of the number of times a literal approaches the Poisson distribution.

To set up the differential equations, we assume for each block of time dt (which can be though of as $1/n$) we choose a pure literal uniformly at random and remove it and its negation. Note that this assumes that $X_0(t) > 0$, and the differential equations do not hold once $X_0(t) \leq 0$. In fact when $X_0 = 0$ the system stops.

It is clear that $\frac{dL}{dt} = -2$, since at each step, two literals are removed. Hence, as $L_0 = 2$, we have $L = 2 - 2t$.

When a random pure literal is chosen, the expected number of times it appears in the formula is simply the average number of clauses a random variable appears in (up to an $O(\frac{1}{n})$ additive error). One can see this by noting that any given pure literal is equally likely to be any of the remaining variables; the fact that its negation appears 0 times does not affect the conditional distribution of its number of appearances, given the current state $(X_0(t), X_1(t), \ldots)$. (The $O(\frac{1}{n})$ discrepancy is caused by the fact that a pure literal is slightly less likely that a random literal to appear 0 times, as we know that one literal, its negation, appears 0 times; this, however, only changes things by an $O(\frac{1}{n})$ term, which can be safely dismissed in the limit as $n \to \infty$. From now on, we ignore this discrepancy in establishing the differential equations.) Hence

$$\frac{dC}{dt} = -A = -\frac{\sum_{i \geq 0} i X_i}{L}.$$

Making use of the identity $Ck = \sum_{i \geq 0} i X_i$, which expresses the total number of remaining variables in the formula in two different ways, and our knowledge of the form of L, we may rewrite this as

$$\frac{dC}{dt} = -\frac{Ck}{2 - 2t},$$

from which it is easily derived that $C = C_0(1 - t)^{k/2}$.

The equations describing the behavior of the X_i are slightly more complex. First, note that the pure literal deleted during a time step appears i times with probability $\frac{X_i}{L}$. Now, suppose the pure literal occurs j times. Then we lose a literal that appears i times whenever one of j clauses containing that variable contains a literal that appears exactly i times. Note that there are $j(k-1)$ variables deleted, as there are $k-1$ variables per clause (1 variable for each clause is taken by the pure literal!). The probability that each such variable is one that appears i times is $\frac{iX_i}{Ck}$. (Again, note that we have here ignored additive $O(\frac{1}{n})$ terms, such as when a two appearances of a literal are deleted.) Hence the expected loss of literals of size i is $-\frac{X_i}{L} - \frac{AiX_i}{Ck}$. One can similarly determine the expected gain in X_i during a time step from all literals that appear $i+1$ times and have 1 appearance deleted. The result yields:

$$\frac{dX_i}{dt} = -\frac{A(k-1)iX_i}{Ck} + \frac{A(k-1)(i+1)X_{i+1}}{Ck} - \frac{X_i}{L} \text{ for } i \geq 1.$$

Note the case of X_0 is special, since we always remove the negation of a pure literal, which by definition appears 0 times, at each step:

$$\frac{dX_0}{dt} = \frac{A(k-1)X_1}{Ck} - \frac{X_0}{L} - 1.$$

3 The Solution

Recall that, once $X_0 = 0$, the process stops. Hence our goal is to determine an explicit equation for X_0, and use it to determine what values of m guarantee that $X_0 > 0$ for $t \in [0, 1)$. Once we have solved this deterministic case given by the differential equations, we can use this information to make statements regarding the limiting case of the random process as $n \to \infty$. (Note that, for technical reasons, we also require $k \geq 3$; see Lemma 4.4 of [1].)

For the equations below, we use $c = \frac{m}{n}$ which is a fixed constant.

One may check that the solutions for the X_i, $i \geq 1$, are given by the following formulas:

$$X_i(t) = \sum_{j=i}^{\infty} \lambda_{i,j} \left(\frac{C}{c}\right)^{j(k-1)/k} (1-t)^{1/2},$$

where

$$\lambda_{i,j} = \frac{2\left(\frac{ck}{2}\right)^j (-1)^{i+j} \binom{j}{i}}{j!}.$$

X_0 can be solved for explicitly, or by noting that $X_0 = L - \sum_{i \geq 1} X_i$, yielding

$$X_0(t) = 2 - 2t - \sum_{i=1}^{\infty} \sum_{j=i}^{\infty} \lambda_{i,j} \left(\frac{C}{c}\right)^{j(k-1)/k} (1-t)^{1/2}.$$

We now find a convenient form for $X_0(t)$:

$$\begin{aligned}
X_0(t) &= 2 - 2t - \sum_{i=1}^{\infty} \sum_{j=i}^{\infty} \lambda_{i,j} \left(\frac{C}{c}\right)^{j(k-1)/k} (1-t)^{1/2} \\
&= 2(1-t)^{1/2} \left[(1-t)^{1/2} - \sum_{i=1}^{\infty} \sum_{j=i}^{\infty} \frac{\left(\frac{ck}{2}\right)^j (-1)^{i+j} \binom{j}{i}}{j!} (1-t)^{(k-1)j/2} \right] \\
&= 2(1-t)^{1/2} \left[(1-t)^{1/2} - \sum_{j=1}^{\infty} \left(\sum_{i=1}^{j} (-1)^{i+j} \binom{j}{i} \right) \frac{\left(\frac{ck(1-t)^{(k-1)/2}}{2}\right)^j}{j!} \right] \\
&= 2(1-t)^{1/2} \left[(1-t)^{1/2} + \sum_{j=1}^{\infty} \frac{\left(\frac{-ck(1-t)^{(k-1)/2}}{2}\right)^j}{j!} \right] \\
&= 2(1-t)^{1/2} \left[(1-t)^{1/2} + \exp\left(\frac{-(1-t)^{(k-1)/2} ck}{2}\right) - 1 \right].
\end{aligned}$$

Hence, to determine when $X_0(t) > 0$, it suffices to examine the expression

$$(1-t)^{1/2} + \exp\left(\frac{-(1-t)^{(k-1)/2} ck}{2}\right) - 1,$$

and to determine the supremum of the set of all c such that this expression is positive for all $t \in [0, 1)$. This can be found by finding the values of c and t such that the above expression is 0 at t and its derivative is 0 at t. This point must satisfy:

$$\begin{aligned} (1-t)^{1/2} + \exp\left(\frac{-(1-t)^{(k-1)/2}ck}{2}\right) - 1 &= 0 \\ \frac{(1-t)^{-1/2}}{2} + \exp\left(\frac{-(1-t)^{(k-1)/2}ck}{2}\right)\frac{ck(k-1)}{4}(1-t)^{(k-3)/2} &= 0 \end{aligned}$$

We use the first equation above to remove the exponential expression from the second by noting that it implies $\exp\left(\frac{-(1-t)^{(k-1)/2}ck}{2}\right) = 1-(1-t)^{1/2}$ and substituting accordingly. The equations can then be solved for c to yield:

$$c = \frac{2}{k(k-1)[(1-t)^{(k-2)/2} - (1-t)^{(k-1)/2}]}.$$

This, in turn, yields a condition on t based solely on k:

$$(1-t)^{1/2} + \exp\left(\frac{-1}{(k-1)((1-t)^{-1/2}-1)}\right) - 1 = 0.$$

This can easily be solved numerically for the correct $t \in [0, 1)$ and in turn for the correct value of c.

Using this framework, we derive Table 1 of values c_k, where c_k is the appropriate threshold for k-SAT formula. That is, c_k is the number such that for any fixed $\epsilon > 0$, if we have a random k-SAT formula with n variables and $(c_k - \epsilon)n$ clauses, with high probability we may find a solution using the pure literal rule, while if we have $(c_k + \epsilon)n$ clauses with high probability the pure literal rule fails to find a solution.

References

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k	c_k
3	1.636938...
4	1.544559...
5	1.403560...
6	1.274162...
7	1.163550...
8	1.069994...
9	0.990510...
10	0.922394...

Table 1: The thresholds for the pure literal rule for k-SAT. These values match simulations quite well even for a very small number of clauses (in the tens of thousands).

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