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The Journal of Logic and Algebraic Programming 47 (2001) 1–14

THE JOURNAL OF LOGIC AND ALGEBRAIC PROGRAMMING

www.elsevier.com/locate/jlap

A sharp threshold for the phase transition of a restricted Satisfiability problem for Horn clauses

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Received 12 April 2000; received in revised form 17 July 2000; accepted 23 August 2000

Abstract

In this paper we examine a variant, *k-HSAT*, of the well-known Satisfiability problem, wherein formula instances are limited to CNF formulae having exactly k literals in each clause at most one of which is un-negated. Such formulae correspond to sets of Horn clauses, each of which involves exactly k propositional variables. In addition, rather than seeking instantiations of the propositional variables that satisfy the formula, satisfying instantiations having at least $k-1$ variables set to 1 are required (such instantiations being referred to as *acceptable*). Viewing formulae as sets of Horn clauses, 'acceptable' instantiations are exactly those that correspond to 'non-trivial' models, i.e., those in which at least one rule has a true antecedent. We show, using analytic methods, that *k-HSAT* exhibits a phase transition whose behavior is significantly different from that of the classical *k-SAT* problem concerning which various researchers have presented empirical evidence for the existence of a constant θ_k such that randomly chosen instances of *k-SAT* on n variables having $m(n)$ clauses are 'almost certainly' satisfiable if $m(n)/n < \theta_k$ and 'almost certainly' unsatisfiable if $m(n)/n > \theta_k$. In this paper we prove a *sharp* threshold result for *k-HSAT for all* fixed $k \geqslant 2$. Specifically, for $\theta_k = (k-1)(k+1)/k!$ it is proved that if ϕ is chosen uniformly at random from instances of *k-HSAT* on n variables and $m(n)$ clauses then

$$\lim_{n\to\infty} \text{Prob}[\phi \text{ has an acceptable instantiation}] = 1 \quad \text{if } \frac{m(n)}{n^{k-1}\log_e n} < \theta_k,$$

$$\lim_{n\to\infty} \text{Prob}[\phi \text{ has an acceptable instantiation}] = 0 \quad \text{if } \frac{m(n)}{n^{k-1}\log_e n} > \theta_k.$$

Keywords: Phase transition; Satisfiability; Horn clause formula

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1. Introduction

The Satisfiability problem, and in particular the restriction of this to propositional formulae in conjunctive normal form with exactly three literals in each clause (3-*SAT*) has been the subject of extensive investigation with respect to the pheonomenon known as a *phase transition*. Informally, this is the behaviour whereby as the number of clauses, m, increases, a 'typical' m-clause instance of 3-*SAT* on n propositional variables progresses from being usually satisfiable to usually unsatisfiable. Furthermore, if one examines this transition in terms of the ratio of number-of-clauses to number-of-variables (m/n) there is an apparent sharp threshold, θ, such that typical instances with $m/n < \theta$ are almost always satisfiable, and typical instances with $m/n > \theta$ are almost always not satisfiable. More formally, if $S(m,n)$ is the proportion of possible instances of 3-*SAT* with n variables and m clauses, that are satisfiable, then experimental studies posit the existence of a threshold θ such that

$$\forall \alpha < \theta \lim_{n \to \infty} |S(\alpha n, n)| = 1,$$

$$\forall \alpha > \theta \lim_{n \to \infty} |S(\alpha n, n)| = 0.$$

The empirical studies presented by Crawford and Auton [6], Larrabee and Tsuji [15] and Selman et al. [17] suggest a value for θ of about 4.24. Analytic methods confirm the existence of a sharp threshold although this has yet to be identified exactly [9]. Some progress, however, has been made in narrowing the region in which such a threshold would have to lie. Thus, initial upper bounds on the clause-to-variable ratio m/n were obtained in Ref. [5] where it was demonstrated that 'almost all' instances with $m/n > 5.19$ are unsatisfiable. This has been improved in Ref. [19] where the bound is lowered to 4.574 building on techniques developed in Refs. [13,14]. A lower bound of 3.003 is proved in Ref. [10], improving the earlier bound of 2.99 given in Ref. [2]. Hence it is known that, for 3-*SAT*, $3.003 \leqslant \theta \leqslant 4.574$. Analytic techniques have proved more successful with 2-*SAT* (which can be decided in time linear in m), the work of Chvátal and Reed [4] and Goerdt [11] proving a sharp threshold at $m/n = 1$ for this problem. An interesting and more general problem is studied, by experimental techniques, in Ref. [18]. In this work the existence of prime implicates of length t in random 3-*SAT* instances is considered: 3-*SAT* being the special case of this problem corresponding to $t = 0$. It is shown that differing value of t induce differing thresholds for the phase transition.

Although the phase-transition phenomenon in 3-*SAT* may be viewed as of purely combinatorial interest, there are, in fact, powerful pragmatic reasons for examining it. The correlation between instances lying close to the threshold region and instances which prove to place the greatest computational demands on heuristic search methods has been observed in empirical studies. A similar correlation is apparent between instances falling at 'extreme' distances from the threshold and instances for which search heuristics can deliver an answer very quickly. Empirical evidence regarding 'threshold effects' in 'hard' combinatorial search problems was first observed by A.I. researchers, notably the studies of Cheeseman et al. [3] and Mitchell et al. [16] on 3-*SAT*, in which exhaustive search strategies were found to divide the space of all possible instances into an 'Easy-Hard-Easy' pattern, with the hardest instances, i.e., those which required the greatest search effort, clustered around some fixed ratio of clauses to variables. These, experimentally observed, connections provide two of the strong practical motivations for investigating phase transitions: instances lying on or close to the threshold provide a natural testbed of 'hard' case with which to evaluate new heuristic methods; and the ease with which 'extreme' instances can often be solved can provide directions for designing efficient (on average) methods for solving some classes of hard, e.g. NP-complete, problems. A classic example of the latter application is the methods of Angluin and Valiant [1] which give fast average-case methods for solving the Hamiltonian cycle problem in graphs with 'sufficiently many' edges. The reader interested in further background on the study of phase-transition phenomena within Pure Mathematics, Artificial Intelligence, and Algorithmics is referred to the survey article in Ref. [7].

The fact that phase-transition phenomena arise in the particular form of satisfiability represented by *k-SAT* and in the more general problem examined in Ref. [18] raises the question of how the transition functions may be affected by considering further restrictions on instances of *k-SAT*. The present paper is concerned with a variant of *k-SAT* but one which can be decided in polynomial time. Furthermore, the specific problem we study is strongly motivated by its implications for Logic Programming. A formal definition of the problem, *k-HSAT*, is given in Section 2, however, in order to provide a preliminary motivation for it we observe that the set of admissible clauses in a given instance of *k-HSAT* is such that at most one literal in each clause may occur in positive form, and it is required that satisfying instantiations set at least $k-1$ variables to the Boolean value 1.

The reason for choosing the restriction to *k-SAT* is that it corresponds to knowledge representation paradigms popular in Artificial Intelligence. Thus the Logic Program paradigm typically restricts itself to logic programs which use the Horn clause. A Horn clause is of the form: $a_1 \leftarrow b_1 \wedge b_2 \wedge \cdots \wedge b_n$, where a_1 is either a positive literal or the empty clause and $b_1, \ldots, b_n$ are positive literals. As is evident, such clauses, when transformed to CNF, limit us to at most one positive literal in each elementary disjunction.

Of course, Logic Programs typically use clauses of a variable length. It is, however, simple to produce an equivalent program where clauses have a fixed length greater than or equal to 3. The length of a clause can be reduced by replacing a pair of variables in that clause by some new variable and adding a clause expressing that the new variable is assigned true if both the replaced variables are assigned true. Each such replacement increases the number of variables and the number of clauses by 1. A clause can be lengthed by padding with Boolean 0s.

Typically also Logic Programs are not restricted to propositional form, but contain logical variables. We can, however, given a program P, consider a program P^* which is obtained by constructing all the ground instances of all the procedures in P obtained by substituting for the logical variables just those terms occurring in the Herbrand universe $H(P)$ constructed from just the constants and functors in P. This move is standard in providing fixpoint semantics for Logic Programs. This will inevitably increase greatly the number of propositional variables and clauses, but shows the relevance of our result to such Logic Programs.

Finally if we consider production rules, another major paradigm used in Artificial Intelligence, we can note that provided, as is typically the case, the rules include no disjunctive conclusions, the set of production rules can be rewritten in the required form by distributing conjunctive conclusions over a set of rules, one for each of the conclusions.

Thus *k-HSAT* is sufficient to express all typical logic programs and production rule bases. A satisfying instantiation for *k-SAT* can be trivially produced by setting all variables to Boolean 0. We therefore require that satisfying instantiations set at least $k-1$ variables to the Boolean value 1, so as to ensure that at least one conclusion can be drawn from the corresponding logic program, which we take as the minimum requirement for such a program to be useful. Thus the threshold we identify distinguishes useful logical programs from those which cannot yield any inference.

The main result of this paper is an analytic proof of a sharp threshold for *k-HSAT*, wherein it is established that the function $r(n,k) = n^{k-1} \log_e n$, has the following property: $\exists \theta_k$, (a constant > 0) such that 'almost all' $m(n)$-clause instances, ϕ, of *k-HSAT*(n) with $m(n)/r(n,k) < \theta_k$ (resp. $m(n)/r(n,k) > \theta_k$) are such that *k-HSAT*$(\phi) = 1$ (resp. *k-HSAT*$(\phi) = 0$). The proof of this result, furthermore, identifies the exact value of θ_k as $(k-1)(k+1)/k!$.

We note here a number of points of interest about these results. Firstly, with the exception of 2-*SAT* in Refs. [3,11], no explicit (as opposed to existential) *sharp* threshold results had been proved analytically for variants of satisfiability: our result not only improves this situation, but also gives the first example of a sequence of sharp threshold results parameterised in terms of the clause length k. A second point is that the analysis uses only established combinatorial mechanisms, such as the 'first-moment' method, and thus raises the possibility that these may be sufficiently powerful to sharpen the threshold for more general problems: a similar indication to this effect was already apparent in Refs. [13,14]. We note here, that Istrate and Ogihara [12] have, independently, considered the phase-transition problem for satisfiability of general Horn clause formulae, i.e., without the restriction that each clause contain exactly k literals, proving that a sharp threshold does not exist for this class.

In the following section we present some basic definitions and the notation used subsequently. In Section 3 the main analytic result on the threshold function for *k-HSAT*(n) is proved. Conclusions and some suggestions for further work are presented in Section 4.

2. Definitions and notation

$\mathbf{X}_n = \langle x_1, x_2, \ldots, x_n \rangle$ denotes a set of n propositional variables. A *literal* is either a variable, x, or its negation $\bar{x}$. In the former case, x is said to be a positive *literal*; in the latter case it is said to be a *negative* literal. A *clause*, s, is a disjunction of literals; s is said to be *trivial* if it contains both the literal x and its negation, and is *non-trivial* otherwise. Similarly, a *product*, p, is a conjunction of literals. A *CNF formula*, ϕ, over $\mathbf{X}_n$ is a conjunction of (non-trivial) clauses $\{s_1, s_2, \ldots, s_m\}$. For any CNF formula, ϕ, f_ϕ denotes the n-variable propositional logic function represented by ϕ. The decision problem *satisfiability* (SAT) asks whether a given CNF formula, ϕ, is such that there exists any instantiation, α, of the propositional variables $\mathbf{X}_n$ of ϕ, for which $f_\phi(\alpha) = 1$. A *k-CNF* fomula is a CNF formula in which every clause has exactly k literals. The decision problem *k-SAT* is the Satisfiability problem restricted to *k-CNF* formulae.

A *rule* is an expression of the form $z \leftarrow y_1 \wedge y_2 \wedge \cdots \wedge y_k$, where $\{y_1, \ldots, y_k\}$ are distinct variables from the set $\mathbf{X}_n$ and z is either the Boolean constant 0 or a variable in $\mathbf{X}_n$. All variables in a rule must be positive and it is assumed that $z \notin \{y_1, \ldots, y_k\}$. If $p = y_1 \wedge \cdots \wedge y_k$, then we may express a rule, $z \leftarrow p$ by the logically equivalent clause, $(z \vee \bar{y}_1 \vee \bar{y}_2 \vee \cdots \vee \bar{y}_k)$.

From the definition of rule it follows that an equivalent clause contains at most one positive literal. We can thus consider the following class of clauses and CNF formulae.

The set of clauses over $\mathbf{X}_n$ containing exactly k literals at most one of which is positive is denoted $HC(n, k)$, The set of *k-CNF* formulae all of whose clauses are in $HC(n, k)$ is denoted $HCNF(n, k)$ with the subset of these that have exactly m clauses denoted $H(n, k, m)$. The decision problem with which this paper is concerned is a variant of *k-SAT* restricted to formulae in $HCNF(n, k)$.

Definition 2.1. *k-HSAT* is the decision problem which takes as input a formula, $\phi \in HCNF(n, k)$ and asks if there is an instantiation, $\alpha \in \{0, 1\}^n$ of $\mathbf{X}_n$ such that $f_\phi(\alpha) = 1$ and *at least* $k - 1$ propositional variables in $\mathbf{X}_n$ are instantiated to 1 under α. If α is an instantiation that certifies an instance ϕ of *k-HSAT*, we say that α is *acceptable* for ϕ. An instance ϕ for which *k-HSAT*(ϕ) holds is said to be *useful.*

A *property*, Π, is a subset of $\bigcup_{n=0}^{\infty} HCNF(n, k)$. A formula $\phi \in HCNF(n, k)$ is said to have property Π if $\phi \in \Pi$. A property is *monotone increasing* if $\phi \in \Pi \Rightarrow \psi \in \Pi$ for all ψ whose clauses are a superset of those in ϕ. Similarly, a property is *monotone decreasing* if $\phi \in \Pi \Rightarrow \psi \in \Pi$ for all ψ whose clauses form a *subset* of those of ϕ. It is easy to see that the property defined by useful instances of *k-HSAT* is monotone decreasing.

3. The sharp threshold for random instances of *k-HSAT*

It may be noted that any instantiation of $\mathbf{X}_n$ in which at most $k - 2$ variables take the value 1 will, trivially, satisfy any $\phi \in HCNF(n, k)$: after setting any subset of at most $k - 2$ variables to 1, any clause will either be satisfied or will have at least one (non-instantiated) negative literal remaining, thus ϕ can be satisfied by assigning all the remaining variables the value 0.

There are, however, good reasons why we should consider such satisfying instantiations as being uninteresting, hence the second condition imposed in Definition 2.1. In particular, the requirement that we have at least $k - 1$ variables assigned the value *true* does not exclude any meaningful knowledge bases. In a knowledge based system, the rules are applicable only if the conditions in the antecedents are satisfied. Even though the falsity of the antecedent guarantees the truth of the rule, it does not justify its inclusion in a knowledge base, since such a rule could never be applied. If fewer than $k - 1$ variables are *true*, no antecedent can be satisfied and so no rule can be applicable and hence the knowledge base as a whole is inapplicable in that situation. Our restriction thus does no more than admit only cases where the corresponding knowledge base has a potential application.

We consider the following two probability distributions on n-variable instances of *k-HSAT*.

(D1) The distribution in which a random formula, denoted subsequently by $F_{n,k,p(n)}$, is chosen by considering each $s \in HC(n,k)$ in turn and including it with probability $p(n)$, excluding it with probability $1 - p(n)$. All such decisions being made independently.

(D2) The distribution in which a random formula denoted subsequently by $G_{n,k,m(n)}$ is chosen uniformly at random from $\mathrm{HCNF}(n,k,m(n))$.

Suppose that $r : (\mathbf{N} \times \mathbf{N} \to \mathbf{R})$ is some (positive) real-valued function. In order to present results regarding phase transitions in k-$HSAT(n)$ we wish to determine: an appropriate function $r(n,k)$ and a constant, θ_k such that,

$$\lim_{n\to\infty} P[G_{n,k,m(n)} \text{ is useful}] = 1 \quad \text{if } \frac{m(n)}{r(n,k)} < \theta_k, \tag{3.1}$$

$$\lim_{n\to\infty} P[G_{n,k,m(n)} \text{ is useful}] = 0 \quad \text{if } \frac{m(n)}{r(n,k)} > \theta_k. \tag{3.2}$$

Distributions similar to $G_{n,k,m(n)}$ are frequently employed in empirical studies. Analysis of this, however, can become rather cumbersome. For this reason our analytic results are derived in terms of $F_{n,k,p(n)}$.

For the analogous random graph distributions ($G_{n,p(n)}$ in which edges are included with probability $p(n)$; resp. $G_{n,m(n)}$ for which an $m(n)$-edge graph is chosen uniformly at random from the set of n-vertex, $m(n)$-edge graphs) it is well known that results obtained, for monotone properties Π, in one distribution may be translated into the other. It is not difficult to show that a similar translation holds when moving from $F_{n,k,p(n)}$ to $G_{n,k,m(m)}$, as we shall demonstrate following the proof of our main theorem which is now stated.

Theorem 3.1. *Let* $p = p(n) = (\log_e n)/n$

$\forall k \geqslant 2$

$$\forall \alpha > k-1 \quad \lim_{n\to\infty} P[F_{n,k,\alpha p} \textit{ is useful}] = 0, \tag{a}$$

$$\forall \alpha < k-1 \quad \lim_{n\to\infty} P[F_{n,k,\alpha p} \textit{ is useful}] = 1. \tag{b}$$

Before presenting the proof of Theorem 3.1, we give an overview of its structure.

A key idea in both parts of the proof is the fact that there is a simple combinatorial characterisation of those $\phi \in HCNF(n,k)$ which are useful.

Let $Q(B,\phi)$ denote the relationship between subsets B of $\mathbf{X}_n$ and k-$HCNF$ formulae ϕ defined by

$$Q(B,\phi) \quad \text{if } |B| \geqslant k-1$$

$$\text{and} \begin{cases} Q1 & \forall\{y_1,\ldots,y_k\} \subseteq B,\ (\bar{y}_1 \vee \bar{y}_2 \cdots \vee \bar{y}_k) \notin \phi, \\ Q2 & \forall\{y_1,\ldots,y_{k-1}\} \subseteq B,\ \forall z \in \mathbf{X}_n - B,\ (\bar{y}_1 \vee \bar{y}_2 \cdots \vee \bar{y}_{k-1} \vee z) \notin \phi. \end{cases}$$

It is not difficult to show that

$$\phi \in HCNF(n,k) \text{ is useful} \iff \exists B \subseteq \mathbf{X}_n : Q(B,\phi). \tag{$*$}$$

It follows from $(*)$ that the probability of $\phi \in F_{n,k,p(n)}$ being useful is equal to the probability of there being a subset B of $\mathbf{X}_n$ for which $Q(B,\phi)$ holds. For Theorem

3.1(a), rather than attempt directly to estimate $P[\exists B \subseteq \mathbf{X}_n : Q(B,\phi)]$ for $\phi \in F_{n,k,p(n)}$ we instead obtain an upper bound on the *expected number* of subsets, B, that satisfy $Q(B,\phi)$ for a random $\phi \in F_{n,k,p(n)}$. Since,

$$P[\phi \text{ is useful}] = P[\exists B : Q(B,\phi)] \leqslant E[|\{B : Q(B,\phi)\}|].$$

Theorem 3.1(a) is proved by showing that the expectation approaches 0 for the stated choices of $p(n)$ and α.

The major part of the proof of Theorem 3.1(a) involves an analysis of the upper bound estimate obtained for $E[|\{B : Q(B,\phi)\}|]$

Proof of Theorem 3.1. *Part* (a): Let

$$\mathrm{Acc}(\phi) =_{\mathrm{def}} \{B \subseteq \mathbf{X}_n : Q(B,\phi)\}.$$

That is, for a given ϕ, $\mathrm{Acc}(\phi)$ is the set of distinct subsets of $\mathbf{X}_n$ that would guarantee that ϕ is useful. For $\phi \in F_{n,k,p}$, $|\mathrm{Acc}(\phi)|$ is a random variable taking values between 0 and $2^n - \mathrm{O}(n^{k-2})$. Letting $E[|\mathrm{Acc}(\phi)|]$ denote the expected value of this random variable with $\phi \in F_{n,k,p}$ a random instance of k-$HSAT(n)$ we have

$$P[\phi \text{ is useful}] \leqslant E[|\mathrm{Acc}(\phi)|]. \tag{3.3}$$

To prove part (a), it suffices to identify $p(n)$ such that $\lim_{n\to\infty} E[|\mathrm{Acc}(\phi \in F_{n,k,p})|] = 0$. The Markov inequality in (3.3) then shows that $\phi \in F_{n,k,p}$ is almost certainly not useful.

$$\begin{aligned} E[|\mathrm{Acc}(\phi)|] &= \sum_{\phi} P[\phi]|\mathrm{Acc}(\phi)| = \sum_{\phi}\sum_{B\subseteq \mathbf{X}_n} P[\phi] I_{Q(B,\phi)} \\ &\qquad \text{(where } I_{Q(B,\phi)} \text{ is the indicator function for the relation } Q) \\ &= \sum_{B}\sum_{\phi} P[\phi] I_{Q(B,\phi)} \leqslant \sum_{B} P[Q(B,\phi)] = \sum_{B} P[B \in \mathrm{Acc}(\phi)]. \end{aligned} \tag{3.4}$$

We thus have, from (3.3) and (3.4)

$$P[\phi \text{ is useful}] \leqslant \sum_{B\subseteq \mathbf{X}_n} P[B \in \mathrm{Acc}(\phi)]. \tag{3.5}$$

The right-hand side of (3.5) is

$$\begin{aligned} \sum_{B\subseteq \mathbf{X}_n} P[B \in \mathrm{Acc}(\phi)] &= \sum_{r=k-1}^{n} \sum_{B\,:\,|B|=r} P[B \in \mathrm{Acc}(\phi)] \\ &\leqslant \sum_{r=k-1}^{n} \binom{n}{r} (1-p)^{\binom{r}{k} + \binom{r}{k-1}(n-r)}. \end{aligned} \tag{3.6}$$

The upper bound in (3.6) follows since, in order for $Q(B,\phi)$ to hold, the condition Q1 forbids $\binom{r}{k}$ clauses in ϕ and the condition Q2 forbids a further $\binom{r}{k-1}(n-r)$ clauses. Simplifying (3.6) using the relationships, $1 + x \leqslant \exp(x)$ and $\binom{n}{r} \leqslant (ne/r)^r$, and combining with (3.5) we obtain

$$P[\phi \text{ is useful}] \leqslant \sum_{r=k-1}^{n} \exp\left(-P\left\{ \binom{r}{k} + n\binom{r}{k-1} - r\binom{r}{k-1} \right\} \right.$$
$$\left. + r\log_e(n/r) + r \right)$$
$$=_{\text{def}} \sum_{r=k-1}^{n} \exp(\beta(r)). \tag{3.7}$$

Substituting $p = \alpha \log_e n/n$ in (3.7), we get

$$\beta(r) = -r\log_e n\left\{ \frac{\alpha}{r}\binom{r}{k-1} + \frac{\alpha}{nr}\binom{r}{k} - \frac{\alpha}{n}\binom{r}{k-1} - 1 + \frac{\log_e r}{\log_e n} - \frac{1}{\log_e n} \right\}$$
$$= -r\log_e n\left\{ \alpha\binom{r}{k-1}\left\{ \frac{1}{r} - \frac{1}{n} \right\} - 1 + \frac{\alpha}{nr}\binom{r}{k} + \frac{\log_e r}{\log_e n} - \frac{1}{\log_e n} \right\} \tag{3.8}$$
$$=_{\text{def}} -r\log_e n\gamma(r). \tag{3.9}$$

So in total we have shown, so far, that

$$P[\phi \text{ is useful}] \leqslant \sum_{r=k-1}^{n} \exp(-r\log_e n\gamma(r)) \tag{3.10}$$

for $\gamma(r)$, which depends on α and n, given in (3.8).

The remainder of the proof of part (a) falls into four parts. If we can show for an appropriate choice of α and all r in the range of the summation that $\gamma(r) > \delta > 0$ (for some fixed δ) then this summation is bounded above by the geometric progression $\sum_{r=k-1}^{n} n^{-\delta r}$ which approaches 0 as n increases. We, thus, complete the proof as follows:

(a1) We show that $\forall k \geqslant 2,\ \forall \varepsilon > 0,\ \exists N_\varepsilon$ such that with $\alpha = k - 1 + \varepsilon,\ \gamma(k-1) > \varepsilon/2k$ whenever $n \geqslant N_\varepsilon$.

(a2) We show that $\forall k \geqslant 2,\ \gamma(r) < \gamma(r+1)$ for $k-1 \leqslant r < s(n,k)$, where $s(n,k) = (k-2)n/(k-1)$ for $k \geqslant 3$, and $2n/((1+\varepsilon)\log_e n)$ for $k = 2$.[1]

(a3) We prove that $\forall k \geqslant 2,\ \gamma(r) > \varepsilon/2k$ for $s(n,k) \leqslant r \leqslant n$.

In combination, (a1)–(a3) allow us to deduce that

$$\forall k \geqslant 2,\ \forall \varepsilon > 0,\ \forall r:\ k-1 \leqslant r \leqslant n,\ \forall n \geqslant N_\varepsilon,\ \gamma(r) > \varepsilon/2k.$$

(a4) Finally, we prove that the geometric progression bounding $P[\phi$ is useful] approaches 0 as n approaches infinity.

Recall that the function $\gamma(r)$ whose behaviour we analyse is

$$\gamma(r) = \gamma\binom{r}{k-1}\left\{ \frac{1}{r} - \frac{1}{n} \right\} - 1 + \frac{\alpha}{nr}\binom{r}{k} + \frac{\log_e r}{\log_e n} - \frac{1}{\log_e n}. \tag{3.11}$$

[1] Strictly speaking, there is no need to consider the case $k = 2$ and $k \geqslant 3$ separately, since, in principle, the method used for the former could be adapted to deal with all k. Such an approach, however, introduces further complications to the analysis due to the form of the binomial coefficients in the definition of $\gamma(r)$ when $k \geqslant 3$. For this reason a more direct approach is used to deal with $k \geqslant 3$, even though this has the disadvantage of dividing the proof into two distinct sections.

Proof of (a1): We wish to show that, $\forall k \geqslant 2$, $\forall \varepsilon > 0$, $\exists N_\varepsilon$ such that with $\alpha = k - 1 + \varepsilon$, $\gamma(k-1) > \varepsilon/2k$ whenever $n \geqslant N_\varepsilon$. We have

$$\begin{aligned}\gamma(k-1) &= \frac{\alpha}{k-1} - \left(1 + \frac{\alpha}{n}\right) + \frac{\log_e(k-1) - 1}{\log_e n} \\ &\geqslant \frac{\varepsilon}{k-1} - \frac{k-1+\varepsilon}{n} - \frac{1}{\log_e n} > \frac{\varepsilon}{2k} \quad \text{when } n \text{ is large enough.}\end{aligned}$$

Proof of (a2): We first deal with the case $k \geqslant 3$. Consider the value of $\gamma(r+1) - \gamma(r)$. From (3.11) this reduces, after basic algebraic manipulations, to

$$\frac{\alpha}{r(r+2-k)}\binom{r}{k-1}\left(k - 2 - \frac{r(k-1)}{n}\right) + \frac{\alpha}{nr(r+1-k)}\binom{r}{k}(k-1) + \frac{\log_e(1+1/r)}{\log_e n}. \tag{3.12}$$

For $k \geqslant 3$ and $k - 1 \leqslant r \leqslant (k-2)n/(k-1)$, the term

$$\frac{\alpha}{r(r+2-k)}\binom{r}{k-1}\left(k - 2 - \frac{r(k-1)}{n}\right)$$

is always non-negative. Since the other terms in (3.12) are positive this establishes (a2) for $k \geqslant 3$.

For the case $k = 2$, we have

$$\gamma(r) = \alpha - \left(1 + \frac{\alpha r}{n}\right) + \frac{\alpha(r-1)}{2n} + \frac{\log_e r}{\log_e n} - \frac{1}{\log_e n}.$$

Substituting $\alpha = 1 + \varepsilon$, this becomes

$$\gamma(r) = \varepsilon - \frac{(1+\varepsilon)r}{2n} - \frac{1+\varepsilon}{2n} + \frac{\log_e r}{\log_e n} - \frac{1}{\log_e n}.$$

Differentiating $\gamma(r)$ with respect to r gives

$$\frac{\mathrm{d}\gamma}{\mathrm{d}r} = -\frac{1+\varepsilon}{2n} + \frac{1}{r \log_e n}.$$

From which we can deduce that $\gamma(r)$ attains its maximal value at $r = 2n/((1+\varepsilon)\log_e n)$, as claimed.

Proof of (a3): For the case $k = 2$, (a2) has established that $\gamma(r) < \gamma(r+1)$ when $1 \leqslant r < 2n/((1+\varepsilon)\log_e n)$, and the value of $\gamma(r)$ decreases subsequently. Given that (a1) establishes $\gamma(1) > \varepsilon/4$ when n is sufficiently large and that the maximum value of r is n, it therefore suffices to show $\gamma(n) > \varepsilon/4$. From (3.11)

$$\begin{aligned}\gamma(n) &= \varepsilon - \frac{1+\varepsilon}{2} - \frac{1+\varepsilon}{2n} + 1 - \frac{1}{\log_e n} \\ &= \frac{1+\varepsilon}{2} - \frac{1+\varepsilon}{2n} - \frac{1}{\log_e n} > \frac{\varepsilon}{4} \quad \text{for } n \text{ large enough.}\end{aligned}$$

For $k \geqslant 3$ and $(k-2)n/(k-1) \leqslant r \leqslant n$, from (3.11) we have,

$$\gamma(r) = \alpha\binom{r}{k-1}\left\{\frac{1}{r} - \frac{1}{n}\right\} - 1 + \frac{\alpha}{nr}\binom{r}{k} + \frac{\log_e r}{\log_e n} - \frac{1}{\log_e n}.$$

This under the conditions stated is

$$\begin{aligned} &\geqslant \frac{\alpha}{n^2}\binom{(k-2)n/(k-1)}{3} + \frac{\log_e((k-2)/(k-1)) + \log_e n - 1}{\log_e n} - 1 \\ &= \Omega(n) \end{aligned}$$

which can be made arbitrarily large.

In summary it has just been proved that for all $\varepsilon > 0$ and n sufficiently large, if we fix $\alpha = k - 1 + \varepsilon$, then $\forall k \geqslant 2,\ \forall r:\ k-1 \leqslant r \leqslant n$, it holds

$$\gamma(r) > \frac{\varepsilon}{2k}. \tag{3.13}$$

Hence, from (3.10),

$$\begin{aligned} P[\phi \text{ is useful}] &\leqslant \sum_{r=k-1}^{n} \exp(-r\log_e n\gamma(r)) \\ &< \sum_{r=k-1}^{n} \exp(-(r\varepsilon/2k)\log_e n) = \sum_{r=k-1}^{n} n^{-\delta r} \\ &\quad (\text{where } \delta = \varepsilon/2k) \\ &= \frac{1-n^{-\delta(n+1)}}{1-n^{-\delta}} - \frac{1-n^{-\delta(k-1)}}{1-n^{-\delta}} \\ &= \frac{n^{-\delta(k+1)} - n^{-\delta(n+1)}}{1-n^{-\delta}} \end{aligned}$$

and since

$$\lim_{n\to\infty} \frac{n^{-\delta(k+1)} - n^{-\delta(n+1)}}{1-n^{-\delta}} = 0$$

we have completed the proof that $\forall k \geqslant 2,\ \forall \varepsilon > 0$, if $\alpha = k - 1 + \varepsilon$ then

$$\lim_{n\to\infty} P[F_{n,k,\alpha p} \text{ is useful}] = 0.$$

Part (b): For part (b), we have a simpler analysis by considering only condition $Q2$ with subsets of size $k-1$. Hence,

$$\begin{aligned} P[\phi \in F_{n,k,\alpha p} \text{ is useful}] &\geqslant P[\exists B : |B| = k-1 \text{ and } \forall z \in \mathbf{X}_n - B(z \vee \bigvee_{x\in B}\bar{x}) \notin \phi] \\ &= 1 - P[\forall B : |B| = k-1, \exists z(z \vee \bigvee_{x\in B}\bar{x}) \in \phi] \\ &= 1 - (P[\exists z(z \vee \bar{x}_1 \vee \cdots \vee \bar{x}_{k-1}) \in \phi])^{\binom{n}{k-1}} \\ &\quad \text{(since the probabilities of individual clauses being chosen are independent)} \\ &\geqslant 1 - (1-(1-\alpha p)^{n-k+1})^{\binom{n}{k-1}} \\ &\geqslant 1 - \exp\left(-\binom{n}{k-1}(1-\alpha p)^{n-k+1}\right). \end{aligned}$$

Substituting $p = (\log_e n)/n$ and noting that

$$\lim_{n\to\infty}\left(1 - \frac{\alpha \log_e n}{n}\right)^{n-k+1} = n^{-\alpha}, \qquad \binom{n}{k-1} \geqslant \frac{n^{k-1}}{(k-1)!} - \mathrm{o}(n^{k-1})$$

we see that the probability of being useful is bounded below by

$$1 - \frac{1}{\exp(n^{k-1-\alpha}/(k-1)!)} - \mathrm{o}(1),$$

hence if $\alpha < k-1$ this probability approaches 1 as n approaches ∞. □

Theorem 3.1 uses the distribution $F_{n,k,p(n)}$, whereas the bulk of empirical studies concerning phase transitions in decision properties of k-*CNF* formulae use an analogue of $G_{n,k,m(n)}$. It is not difficult to show that we can translate our sharp threshold obtained in $F_{n,k,p(n)}$ to one in terms of $G_{n,k,m(n)}$. With such a translation we prove the result stated in the abstract.

Theorem 3.2. *Let* $\theta_k = ((k-1)(K+1))/k!$

$$\text{(a)}\ \lim_{n\to\infty} \mathrm{Prob}[\phi \in G_{n,k,m(n)}\ \textit{is useful}] = 1 \quad \textit{if}\ \ \frac{m(n)}{n^{k-1}\log_e n} < \theta_k,$$

$$\text{(b)}\ \lim_{n\to\infty} \mathrm{Prob}[\phi \in G_{n,k,m(n)}\ \textit{is useful}] = 0 \quad \textit{if}\ \ \frac{m(n)}{n^{k-1}\log_e n} > \theta_k.$$

Proof. The argument given in Ref. [1], establishes that if Π is some monotone decreasing property of n-vertex graphs and $p_0(n)$, $p_1(n)$ are such that

$$\lim_{n\to\infty} P[G_{n,p_0(n)} \in \Pi] = 0,$$
$$\lim_{n\to\infty} P[G_{n,p_1(n)} \in \Pi] = 1,$$

then choosing

$$M_0(n) \geqslant \binom{n}{2} p_0(n)(1+\beta(n)),$$
$$M_1(n) \leqslant \binom{n}{2} p_1(n)(1-\beta(n)),$$

gives

$$\lim_{n\to\infty} P[G_{n,M_0(n)} \in \Pi] = 0,$$
$$\lim_{n\to\infty} P[G_{n,M_1(n)} \in \Pi] = 1,$$

here

$$\beta(n) = \mathrm{O}\left(\log n \Big/ \left(\binom{n}{2} p(n)\right)^{0.5}\right).$$

The argument is based on the fact that the expected number of edges of $G \in G_{n,p(n)}$ is $M(n) = \binom{n}{2}p(n)$. In Ref. [1] if $G \in G_{n,p(n)}$ has less than (resp. more than) $M(n)(1+\beta(n))$ (resp. $M(n)(1-\beta(n))$) edges, then a suitable number of edges are randomly added (resp. removed) to give a (random) graph G^*. By using standard bounds on the tail of the Binomial distribution, see e.g. Ref. [8], it is easily shown that $P[G^* \in \Pi]$ is 'close to' $P[G_{n,p(n)} \in \Pi]$.

In order to prove Theorem 3.2, it suffices to observe that the relationship proved in Ref. [1] is based on properties of the Binomial distribution, i.e., not on the fact that *graph*-theoretic properties per se are addressed.

Thus, we may employ a similar argument with $|HC(n,k)| = \binom{n}{k}(k+1)$ playing the rôle of $\binom{n}{2}$ (the latter corresponding to the maximum number of possible edges in an n-vertex graph).

From Theorem 3.1(a), we have $P_0(n) = \alpha \log_e n/n$ for $\alpha > k-1$, from which we deduce that if

$$M_0(n) \geqslant |HC(n,k)|p_0(n)\left(1 + \mathrm{O}\left(\frac{\log n}{(|HC(n,k)|p_0(n))^{0.5}}\right)\right)$$

then

$$\lim_{n\to\infty} P[\phi \in G_{n,k,M_0(n)} \text{ is useful}] = 0.$$

Since

$$M_0(n) = \frac{\alpha(k+1)}{k!} n^{k-1} \log_e n\left(1 + \mathrm{o}\left(\frac{\log n}{n^{k-1}}\right)\right)$$

setting $\theta_k = (k-1)(k+1)/k!$ gives part (a) of Theorem 3.2.

A similar argument using $p_1(n) = \alpha \log_e n/n$ for $\alpha < k-1$, and

$$M_1(n) \leqslant |HC(n,k)|p_1(n)\left(1 + \mathrm{o}\left(\frac{\log n}{n^{k-1}}\right)\right)$$

proves part (b). $\square$.

4. Conclusions and further work

In this paper a variation of *k-SAT* – *k-HSAT* – which is motivated by a natural application in Logic Programming has been considered with respect to its phase-transition behaviour. Through the use of purely analytic methods a complete characterisation of the phase-transition threshold, for all constant $k \geqslant 2$ has been obtained.

One question of (largely combinatorial) interest concerns the *rate* at which the transition from $p_1(n)$ (the 'almost surely' positive random instances) to $p_0(n)$ ('almost surely' negative random instances) occurs. Notice that the interval $[p_1(n), p_0(n)]$ must contain the so-called *critical probability*, $\chi(n)$, for which

$$P[\phi \in F_{n,k,\chi(n)} \text{ is useful}] = 0.5.$$

The analysis of Theorem 3.1 shows that $\chi(n)$ is about $(k-1)\log_e n/n$. This was argued, however, by showing that for any $\varepsilon > 0$, $p(n) = (k-1\pm\varepsilon)\log_e n/n$ 'almost surely' determines whether random instnaces in $F_{n,k,p(n)}$ are useful or otherwise. Thus for any *constant* $\varepsilon > 0$, the transition from 'almost certainly' positive to 'almost certainly' negative occurs in an interval of length at most $2\varepsilon \log_e n/n$. Friedgut and Kalai [9] present a rather stronger definition of a property having a 'sharp' threshold, namely:

Let Π be a monotone graph property. For $\alpha \in \{0, 1\}$, let $p_\alpha(n)$ be such that

$$\lim_{n \to \infty} P[G_{n,p_\alpha(n)} \in \Pi] = \alpha$$

and $\chi(n)$ be such that $P[G_{n,\chi(n)} \in \Pi] = 0.5$. Π has a *sharp threshold* (in the sense of [9]) if

$$\lim_{n \to \infty} \frac{|p_1(n) - p_0(n)|}{\chi(n)} = 0. \tag{4.1}$$

In other words the length of the transition interval is asymptotically less than the critical probability.

It is natural to ask whether *k-HSAT* has a sharp threshold under the stronger definition given by (4.1): the proof of Theorem 3.1, only gives the limit in (4.1) as 2ε for any constant ε. In fact, as the reader may verify, closer inspection of the proof shows that all of the analysis continues to hold if we replace $\varepsilon > 0$ (constant) by $\varepsilon(n) \geqslant 1/f(n)$ *provided that* $f(n) = \mathrm{o}(\log n)$ (for $f(n) = \Omega(\log n)$ the analyses of neither (a1) nor part (b) are valid). It follows that the length of the transition interval is $(2/f(n))(\log_e n/n)$ for any $f(n) = \mathrm{o}(\log n)$. Combining this with the critical probability $\chi(n) \approx \log_e n/n$ in (4.1), we now get $\lim_{n\to\infty}(2/f(n))$ which is 0. Thus, *k-HSAT does* have a sharp threshold within the stronger sense introduced in Ref. [9]. It remains open as whether prove a 'narrower' transition interval holds, e.g. $\mathrm{O}(1/n^x)$ for some $x > 0$.

Of more immediate interest are the questions that arise from our definition of *k-HSAT*. The concept of an instance ϕ being useful is motivated by the use of Horn clauses to represent knowledge in KBS: thus the *k-HCNF* equivalent to a rule base $R = \{z_i \leftarrow p_i\}$ is useful if there is a consistent model for R in which *at least one* of the antecedents z_i is true. While this is arguably a minimal requirement for a knowledge base to be 'useful', in practice one might well wish for rather more. Some possible further requirements may, informally, be phrased as

(R1) The knowledge-base contains no 'inactive' rules $z_i \leftarrow p_i$, that is, for each rule, $z_i \leftarrow p_i$ there is *some* consistent model for R for which the antecedent z_i is true.

(R2) There is a consistent model under which at least *some given proportion*, ρ, of the rules have antecedents which are *all* true in the model.

(R3) There are at least some number $\delta(n, k)$ of useful models from the $2^n - \mathrm{O}(n^{k-2})$ possible.

It is worth remarking that with the exception of (R1) for which there is an obvious polynomial-time decision method, the computational-complexity of the associated decision problems for (R2) and (R3) is less clear, and it would be of interest to know under what conditions (on ρ and δ) these problems have polynomial-time algorithms.

In the context of the present paper, the properties defined by (R1) and (R3) are easily seen to be monotone decreasing and examining how the additional constraints affect the phase-transition offers one area for further work. If, as seems plausible, (R3) is intractable (say for $\delta(n, k) \approx c2^n$ for constant $0 < c < 1$), analysis of phase-transition behaviour may well-provide valuable insight into the development of methods which perform well 'on average'.

Acknowledgements

The work reported in this paper was carried out with support from EPSRC Grant GR/L/77089.

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