DIMENSION-DEPENDENT BEHAVIOR IN THE SATISFIABILITY OF RANDOM
K-HORN FORMULAE

GABRIEL ISTRATE∗

Abstract. We determine the asymptotical satisfiability probability of a random at-most-\(k\)-Horn formula, via a
probabilistic analysis of a simple version, called PUR, of positive unit resolution. We show that for \(k = k(n) \to \infty\)
the problem can be “reduced” to the case \(k(n) = n\), that was solved in [17]. On the other hand, in the case \(k = \text{constant}\)
the behavior of PUR is modeled by a simple queuing chain, leading to a closed-form solution when \(k = 2\).
Our analysis predicts an “easy-hard-easy” pattern in this latter case. Under a rescaled parameter, the graphs of
satisfaction probability corresponding to finite values of \(k\) converge to the one for the uniform case, a “dimension-
dependent behavior” similar to the one found experimentally in [20] for \(k\)-SAT. The phenomenon is qualitatively
explained by a threshold property for the number of iterations of PUR makes on random satisfiable Horn formulas.
Also, for \(k = 2\) PUR has a peak in its average complexity at the critical point.

Key words. random Horn satisfiability, critical behavior, probabilistic analysis.

AMS subject classifications. 68Q25,82B27

1. Introduction. Finding the ground state (state of minimum energy) of a physical system and computing an optimal solution to a combinatorial optimization problem are intuitively two very similar tasks. This simple observation, that motivated the development of simulated annealing [19], a simple general-purpose heuristic for combinatorial optimization, lies behind the recent birth of a new field at the crossroads of Statistical Mechanics, Theoretical Computer Science and Artificial Intelligence, that studies phase transitions in combinatorial problems (see [14] for a readable introduction). The transfer of principles and methods from Physics (mainly from Spin Glass Theory [25]) to Computer Science has already been quite successful, and is responsible for a couple of interesting results, such as a better understanding of the factors that account for computational intractability [27, 28], strikingly accurate predictions of the average running time of various algorithms [11, 21], or of expected values of optimal solutions [23].

The need for a rigorous validation of these insights is quite obvious. The theory of spin glasses is a relatively young field, which still presents many heuristic, unsolved or plain controversial aspects (for example see [25, 31, 30] for a debate on the validity and scope of the so-called Parisi solution of the Sherrington–Kirkpatrick model). Moreover, while physical intuition can guide the development of the theory for “physical” models, by corroborating (or falsifying) some of its predictions (e.g. see [25], for a discussion of the demise, on physical grounds, of the first formulation of the so-called replica method), such intuition is not available when applying this type of ideas to combinatorial problems. Given that rigorous results are hard to come by in the case of spin glasses proper, it is not surprising that while there has been recently some progress (see e.g. [33]), an analysis of most interesting combinatorial problems is still out of reach.

An approach that was popular in Statistical Mechanics was to gather intuition through the systematic study of exactly solved models [4]. These are “toy” versions of the original models that are simple to deal with, but retain much of the properties of the former ones. We advocate such an approach for problems in Computer Science as well, and the purpose of this paper is to present a (hopefully nontrivial) “exactly solvable satisfiability model” that displays a dimension-dependent behavior fairly similar to the one observed previously in various contexts such as percolation [3], self-avoiding walks, and recently for \(k\)-satisfiability.

∗ Center for Nonlinear Science and CIC-3 Division, Los Alamos National Laboratory, Los Alamos, NM 87545, gistrate@cnls.lanl.gov
by Kirkpatrick and Selman \[20\]. The problem we investigate is \textit{random Horn satisfiability}, and the “dimensionality” of a formula is taken to be the \textit{maximum length} of its clauses.

\section{Overview.} There are actually two different notions of phase transition in a combinatorial problem. The first of them, called \textit{order-disorder phase transition} applies to optimization problems and directly parallels the approach from Statistical Mechanics. Potential solutions for an instance of $P$ are viewed as “states” of a system. One defines an abstract \textit{Hamiltonian (energy) function}, that measures the “quality” of a given solution, and applies methods from the theory of spin glasses \[25\] to make predictions on the typical structure of optimal solutions. In this setting a phase transition is defined as non-analytical behavior of a certain “order parameter” called free energy, and a discontinuity in this parameter, manifest by the sudden emergence of a \textit{backbone} of constrained “degrees of freedom” \[27\] is responsible for the exponential slow-down of many natural algorithms.

The second definition is combinatorial and pertains to decision problems. It relies on the concept of \textit{threshold property} from random graph theory, more precisely a restricted version of this notion, called \textit{sharp threshold}. A satisfiability threshold always exists for monotone problems \[7\], but may or may not be sharp (we speak of a \textit{coarse threshold} in the latter case).

The layout of the paper is as follows: in section 3 we review the results of Kirkpatrick and Selman, in particular discussing the concept of \textit{critical behavior}, as well as some objectionable aspects of their results. We then define the type of dimension dependent behavior we are interested in, argue that it captures to a large extent the results presented in \[20\], and contrast it with critical behavior. Our results are presented and discussed in section 6, while in section 14 we further discuss their significance.

Finally for $k = 2$, the one where the satisfaction probability has a singularity we are able to rigorously display another phenomenon that is believed to be characteristic of phase transitions: in many cases the “hardest on the average” instances appear at the transition point (even if we only consider satisfiable instances \[1\] \[16\]); this feature is quite robust with respect to the choice of the particular algorithm \[8\]. We are able to prove that for a \textit{particular problem}, random at-most-2-Horn satisfiability, the average running time of a \textit{particular algorithm}, when restricted to satisfiable instances (the ones that are statistically significant on both sides of the critical point) is finite outside the critical point, and it diverges as we approach this point, thus providing some evidence for the experimental wisdom.

\section{Phase transitions and critical behavior.} We first discuss, briefly and limited to our interests, threshold phenomena. Perhaps the best way to introduce them is through a concrete example. To do this, we will use one “canonical” NP-complete problem, \textit{k-CNF satisfiability}.

To generate random formulas we use a model with one parameter, the \textit{constraint density} $c$, defined as the ratio between the number of clauses $m$ and the number of variables $n$ of the formula. A random formula is obtained by choosing $m$ random clauses. If we plot the probability that such a random formula is satisfiable against the constraint density $c$, we notice the existence of a critical value $c_k$ such that the satisfaction probability drops (as $n \rightarrow \infty$) from one to zero at $c_k$. Such a “sudden change” is an illustration of the mathematical concept of \textit{sharp threshold}, qualitatively illustrated in Figure 3. The existence of a critical value $c_k$ has not been rigorously established (except for $c_2 = 1$), even though Friedgut \[9\] has shown that the transition is “sharp” for every $k$.

Of special interest will also be the width of the so-called \textit{scaling window} (a.k.a. \textit{critical region}). To define it consider, for $0 < \delta < 1$, $\alpha_+ (n, \delta)$, the supremum over $\alpha$ such that for $m = \alpha n$, the probability of a random formula being satisfiable is at least $1 - \delta$. Similarly, let

\footnote{For technical convenience, all over the paper \textit{random k-Horn satisfiability} is understood as \textit{random at-most-k-Horn satisfiability}.}
\( \alpha_+(n, \delta) \) be the infimum over \( \alpha \) such that for \( m = \alpha n \), the probability of a random formula being satisfiable is at most \( \delta \). Then, for \( \alpha \) within the \( \delta \)-scaling window

\[
W(n, \delta) = (\alpha_-(n, \delta), \alpha_+(n, \delta)),
\]

the probability that a random formula is satisfiable is between \( \delta \) and \( 1 - \delta \).

We will be interested in the width of the window \( W(n, \delta) \) as a function of \( n \). It is generally believed that \( |W(n)| = \theta(n^{-1/\nu}) \) for some \( \nu = \nu_k \geq 1 \) independent of \( \delta \), even though the existence of \( \nu_k \) has only been established for \( k = 2 \) [6].

3.1. Order/disorder phase transitions. Statistical mechanics deals with the description of systems having a large number of degrees of freedom. One of its fundamental predictions concerns the fact that at thermal equilibrium each such state occurs with probability proportional to \( \exp(-\beta H(\sigma)) \), where \( \beta \) is an inverse temperature, and \( H \) is a Hamiltonian function, describing the energy of the particular state \( \sigma \). The resulting distribution is called the Gibbs distribution \( G_\beta \) given by

\[
\Pr[\sigma] = \frac{\exp(-\beta \cdot H(\Phi; \sigma))}{Z[\Phi]},
\]

where

\[
Z[\Phi] = \sum_{\sigma \in \{0,1\}^n} \exp(-\beta \cdot H(\Phi; \sigma))
\]

is the so-called partition function.

Changes in the order properties of the system, which characterize order-disorder phase transitions, manifest themselves as non-analytical behavior of thermal averages (i.e. averages over the Gibbs distribution) of a certain order parameter. We want to emphasize that the physicists’ use of the term order parameter would be quite different from the one from combinatorics. An order parameter is a quantity that is zero on one side of the phase transition and becomes non-zero on the other side (for instance the satisfaction probability could be an order parameter).
One of the simplest illustrations of these concepts is the two-dimensional Ising model (see [4] for a thorough treatment). In this model we have a number of spins, that are small magnets located on the vertices of the two-dimensional lattice, and pointing either up or down. The spins interact with their neighbors and with an external magnetic field \( h \in \mathbb{R} \), which will tend to align the spins in one of the two directions. The energy of a state \( \sigma \) is

\[
H(\sigma) = -\sum_{i \sim j} \sigma_i \cdot \sigma_j + h \cdot \left( \sum_i \sigma_i \right).
\]

The order parameter is called free energy, is a function of temperature, and is formally defined as

\[
f = -\frac{1}{\beta n} \ln Z[\Phi].
\]

It measures the fraction of spins that are “frozen” when the field is turned off.

We now briefly describe the essence of the phase transition: above a certain temperature \( T_c \), the Curie-Weiss point, when the magnetic field is turned to zero the proportion of spins that point in each direction is about \( \frac{1}{2} \) (the so-called disordered phase). But for temperatures below \( T_c \) when we turn the field to zero some orientation still dominates (the ordered phase), and the proportion of spins pointing up(down) changes discontinuously as \( h \) passes through zero.

The connection with combinatorial optimization follows from the observation that when \( \beta \to \infty \) (that is the temperature approaches 0 K), the Gibbs distribution \( G_\beta \) converges to a uniform distribution \( G \) on the set of states of minimal energy (ground states). Thus, based on this analogy, one can hope that ideas from Statistical Mechanics are able to provide insight into the structure of optimal solutions to an instance of a problem in Combinatorial Optimization. Rather than providing a complete discussion (which would require to rigorously define the notion of optimization problem) we will discuss this in the context of MAX 3-SAT, the optimization version of satisfiability. For now it suffices to mention the three main ingredients of an optimization problem, its instances, solutions to instances of a problem, and an cost function, that measures the quality of a solution for a certain instance.

**Example 1.** (MAX 3-SAT)

**Input:** A propositional formula \( \Phi \) in conjunctive normal form, such that every clause has length exactly 3.

**Solution:** A truth assignment \( \sigma \) for the propositional variables in \( \Phi \) that maximizes the number of satisfied clauses.

**Cost function:** The cost \( C(\Phi, \sigma) \) of a truth assignment \( \sigma \) for an instance \( \Phi \) of MAX 3-SAT is the number of clauses of \( \Phi \) that are violated by \( \sigma \).

Let \( Q \) be an optimization problem and let \( \Phi \) be an instance of \( Q \) “on \( n \) variables” (i.e., all solutions have length \( n \)). We view the set of all assignments on \( \{0, 1\}^n \) as “states of a system.” To each such state \( \sigma \) we associate the Hamiltonian (energy function)

\[
H(\Phi; \sigma) = \text{the cost of instance } (\Phi; \sigma) \text{ of } Q.
\]

**Example 2.** Let \( \Phi \) be a 3-CNF formula, and let \( \sigma \) be an assignment. According to the previous definition \( H(\Phi; \sigma) = C(\Phi; \sigma) \). \( H \) can be formally expressed \([26]\) as

\[
H(\Phi; \sigma) = \sum_{i=1}^{m} \delta \left[ \sum_{i=1}^{n} C_{\ell,i} \cdot (-1)^{\sigma_i} - 3 \right],
\]
where $\delta[i; j] = 1_{i=j}$ is the Kronecker symbol and $C_{l,i}$ is 1 if the $l$\textsuperscript{th} clause contains the literal $x_i$, $-1$ if it contains $\overline{x_i}$ and zero otherwise.

For the case of problems of interest to Computer Science the instance $\Phi$ is not fixed, but rather is a sample from a certain distribution. This is very similar to the context of spin-glass theory, a subfield of Statistical Mechanics. The extra ingredient of this theory is that the coupling coefficients are no longer considered fixed, but are rather independent samples from a certain distribution. In the language of the theory of spin glasses $\Phi$ is called a \textit{quenched quantity}.

As in the case of the Ising model, the order parameter is the \textit{ground state free energy}, more precise its expected value

$$\overline{f} = -\frac{1}{\beta_n} \ln(\mathcal{Z}),$$

where $\langle \ldots \rangle$ stands for the average over the random distribution of $\Phi$.

\textbf{Definition 3.1.} A physical (order/disorder) phase transition in a combinatorial optimization problem is a point where $\overline{f}$ is not analytical.

Free energy has an especially crisp intuitive interpretation in the case of the problem MAX 3-SAT $\mathbb{P}^3$.

\textbf{Example 3.} Let $\Phi_n$ be an instance of MAX 3-SAT, let $A$ be the set of optimal assignments to $\Phi_n$, endowed with the uniform measure $\mu_n$. Statistical Mechanics predicts that, as $n \to \infty$, $\mu_n$ is “close” to a product measure on $\{0, 1\}^n$, $\mu_{1,n} \ldots \mu_{n,n}$. The free energy per site $f$ is the fraction of variables $x_i$ that are (asymptotically) fully constrained (that is $\mu_{i,n}$ converges in distribution to a measure having all its weight on one of the two points 0,1.

4. Critical behavior and the mean-field approximation. An important feature that order/disorder phase transition share with the combinatorial notion of \textit{threshold properties} (that are usually the type of phase transition of interest in combinatorics) is that the various quantities of interest, such as the satisfaction probability, the ground state energy, and the location of the phase transition are hard to compute. No general-purpose methods exist, and in some cases even obtaining good non-rigorous estimates is a challenging open problem.

A technique that often provides realistic approximate values for these quantities came to be known as the \textit{mean-field (annealed) approximation}. In a nutshell a mean-field approximation assumes that we are trying to compute the average (over a certain discrete probability space) of a certain expression $f \circ (g_1, \ldots, g_n)$. Then the mean field-approximation amounts to taking

$$E[f(g_1(x), \ldots, g_n(x)] \sim f[E[g_1(x)], \ldots, E[g_n(x)]].$$

This technical definition of the mean-field approximation does not convey a useful intuition: suppose we want to solve a combinatorial problem whose objective function depends on simultaneously satisfy several “constraints” whose effects are usually not independent. The mean-field approximation ignores the dependencies between various constraints, and treat them as independent.

\textbf{Example 4.} Let us return to the case of spin glasses. Each configuration of spins $\sigma$ has an energy specified by a Hamiltonian $H(\sigma)$. A typical expression for $H(\sigma)$ is

$$H(\sigma) = \sum_{i \sim j} a_{i,j}\sigma_i\sigma_j,$$
where the $a_{i,j}$’s are interaction coefficients between adjacent spins (according to some adjacency graph specific to the considered model). The quantity of interest, average free energy $\mathcal{F}$ is hard to compute directly because of the logarithmic function present in the definition of the free energy. In this context the mean-field approximation amounts to

$$\mathcal{F} \sim -\frac{1}{\beta n} \ln[Z(\Phi)].$$

The advantage of this heuristic is that the average on the right-hand side is one that is usually much easier to compute.

For combinatorial phase transitions, the mean-field approach usually amounts to an approximation using the so-called first-moment method

**Example 5. ($k$-Satisfiability)**

The reason that the satisfiability probability of a random formula is hard to compute is that, for two assignments $A, B$ the events $A \models \Phi$ and $B \models \Phi$ are not independent. One way to construct a mean-field theory for $k$-SAT is to ignore the dependencies between these events. More precisely, we have

$$1_{SAT}[\Phi] = f(g_{A_1}[\Phi], \ldots, g_{A_2^n}[\Phi]),$$

where

$$f(x_1, x_2, \ldots, x_{2^n}) = 1 - \prod_{i=1}^{2^n} x_i,$$

and

$$g_A[\Phi] = \begin{cases} 1, & \text{if } A \not\models \Phi, \\ 0, & \text{otherwise}. \end{cases}$$

Define $\gamma_k = 1 - 2^{-k}$. The mean-field approximation amounts to

$$\Pr[\Phi \in SAT] = \mathbb{E}[1_{SAT}[\Phi]] \sim f(\mathbb{E}[g_1[\Phi]], \ldots, \mathbb{E}[g_{2^n}[\Phi]])$$

Since

$$\mathbb{E}[g_1[\Phi]] = \ldots = \mathbb{E}[g_{2^n}[\Phi]] = 1 - \gamma_k^{cn}$$

this reads,

$$\Pr[\Phi \in SAT] \sim 1 - [1 - \gamma_k^{cn}]^{2^n} \sim 1 - e^{-2^n \gamma_k^n} = 1 - e^{-\mathbb{E}[\#SAT[\Phi]]}$$

where $\#SAT[\Phi]$ is the number of satisfying assignments for $\Phi$. Thus (neglecting the case $\mathbb{E}[\#SAT[\Phi]] = 1$)

$$\Pr[\Phi \in SAT] = \begin{cases} 1, & \text{if } \mathbb{E}[\#SAT[\Phi]] \to \infty, \\ 0, & \text{if } \mathbb{E}[\#SAT[\Phi]] \to 0. \end{cases}$$
4.1. Critical exponents and behavior. A phenomenon that has been observed in various contexts is critical behavior. In these cases the class of problems under study has an intrinsic notion of dimensionality $d$, and in the limit $d \to \infty$ (or sometimes even when $d$ is greater than a so-called critical dimension) “the annealed approximation becomes exact”.

A way to give precise meaning to the above quote comes from the concept of universality. In Statistical Mechanics one define certain critical exponents, that describe the behavior of the system near the critical points; universality predicts that phase transitions with the same critical exponents are “structurally similar”.

Since critical exponents can be defined for the mean-field versions of the physical models too, critical behavior means that as $d \to \infty$ (or, sometimes, for $d$ larger than a value called the upper critical dimension) the critical exponents of the $d$-dimensional system coincide with the critical exponents of the $d$-dimensional mean-field model.

**Example 6.** (Bond) percolation on the lattice $\mathbb{Z}^d$. Percolation \cite{12} is a mathematical theory that models the flow of liquids in random porous media. In our case the flow is on the lattice $\mathbb{Z}^d$ of dimension $d$, and the model has one parameter, the edge probability $p \in [0, 1]$. Each bond (grid edge of the lattice $\mathbb{Z}^d$) is considered open with probability $p$ (independently of the other bonds) and the order parameter is the probability $P_d(p)$ that the origin lies in an infinite cluster. $P_d$ is a monotonically increasing function of $p$. It is believed that $P_d(p)$ is zero up to a critical value $p_c(d)$ (known rigorously only for $d = 2$), greater than zero beyond that point, and non-analytical but continuous (at least for $d = 2$) at $p_c(d)$. It is also believed that above (and around the critical value) $P_d(p) \sim (p - p_c(d))^\beta$ where $\beta$ is a critical exponent that depends on $d$ but not on the explicit lattice considered (i.e. it would be the same if we choose another $d$-dimensional lattice instead of $\mathbb{Z}^d$). This is only one of the several critical exponents that are believed to structurally characterize percolation on $d$-dimensional lattices (see \cite{12}).

Without going into further details, we note that the “mean-field approximation” corresponds to considering percolation on the $d$-dimensional Bethe lattice, and the critical behavior amounts to the observation that for $d$ greater than a critical dimension (known to be at most 16 \cite{13}, and is believed to be 6) the critical exponents of percolation on $\mathbb{Z}^d$ are those of percolation on the Bethe lattice.

4.2. Rescaling and critical behavior. A recent example of critical behavior has recently been observed experimentally by Kirkpatrick and Selman \cite{20} for satisfiability problems.

Their results do not mention critical exponents (although it is closely related). To explain them, we need to introduce first another concept from Statistical Mechanics: finite-size scaling. The intuition behind it is that \cite{20} “sufficiently close to a threshold or critical point, systems of all sizes are indistinguishable except for an overall change of scale.” In mathematical terms this amounts to defining a new order parameter that “opens up” the scaling window, the region where the probability decreases from 1 to 0.

**Example 7.** Hamiltonian Cycle.

The random model has one parameter $m$, the number of edges. A random sample is obtained by choosing uniformly at random a set of $m$ distinct edges of a complete graph with $n$ vertices. The following result (obtained by Komlóss and Szemerédi \cite{22}) describes the phase transition in this problem:

Let $m = m(n) = \frac{1}{2} n \cdot \log(n) + \frac{1}{2} n \cdot \log \log(n) + c_n \cdot n$. Then
\[ \lim_{n \to \infty} P r[ G \text{ has a Hamiltonian cycle}] = \begin{cases} 
 0, & \text{if } c_n \to -\infty, \\
 e^{-e^{-2c}}, & \text{if } c_n \to c, \\
 1, & \text{if } c_n \to \infty. 
\end{cases} \]

A rescaled parameter for the Hamiltonian cycle problem can be defined by \( c_n = \frac{1}{n} \cdot \left[ m - \frac{1}{2} n \cdot \log(n) - \frac{1}{2} n \cdot \log \log(n) \right] \). This parameter yields a rescaled limit probability function \( f(c) = e^{-e^{-2c}} \).

It is important to note that, since an annealed approximation yields an expression for the order parameter (in our case satisfaction probability) that will usually display a phase transition as well, a rescaled parameter can be defined for the mean-field version of the problem as well.

The definition of the rescaled parameter allows a precise formulation of the intuition that an annealed approximation becomes exact in the limit \( d \to \infty \). Let \( P_d \) be a class of satisfiability problems indexed by a dimensionality parameter \( d \), let \( F_d \) be the rescaled satisfaction probability graph of \( P_d \), and let \( F_{\text{ann},d} \) be the rescaled graph corresponding to the annealed approximation. Kirkpatrick and Selman observe experimentally that as \( d \to \infty \), the function sequences \( F_d, F_{\text{ann},d} \) converge punctually to a common limit \( F_{\infty} \).

**Example 8.** We present in detail the experimental results of Kirkpatrick and Selman. They define an (approximate) rescaled parameter for \( k \)-SAT

\[ y_k = n^{1/\nu_k} \frac{(c - c_k)}{c_k}, \]

where \( c = m/n \), \( c_k \) is the critical threshold for \( k \)-SAT, and \( \nu_k \) is the scaling width coefficient. Also, define the “annealed rescaled parameter”

\[ y_{\infty,k} = n \frac{(c - c_k)}{c_k}, \]

The rescaled limit probability graphs (and, see below, the rescaled versions of the mean-field versions) seem to converge (see Fig. 4 in that paper) to the “annealed limit”

\[ f_{\infty}(y) = e^{-2^{-y}}. \]

**Definition 4.1.** In this paper dimension-dependent behavior refers to the above-mentioned type phenomenon, convergence of the “rescaled” probability functions (and their annealed counterparts) to some common annealed limit.

**Observation 1.**

It is important to note that dimension-dependent behavior is at the same time more and less demanding than critical behavior.

It is more demanding since it requires that the annealed approximation be exact throughout the (rescaled version) of the critical region. In contrast, critical exponents only provide a
qualitative picture of this region, rather than uniquely determine the limit probability throughout it; for instance the width of the scaling window \( \nu \) is equal to \( 2\beta + \gamma \), where \( \beta \) is the so-called order-parameter exponent, that characterizes the asymptotic behavior of the order parameter close to the transition point, and \( \gamma \) is called susceptibility exponent (see e.g. [6]). It is less demanding since it does not assume the existence of critical exponents, therefore it makes sense for problems having coarse thresholds, including those that have no singular/critical points.

Why should we expect critical behavior and the above form for the annealed limit? The intuition is very simple: the major difficulty in computing the probability that a random \( k \)-SAT formula is satisfiable is the fact that, for two assignments \( A \) and \( B \), the events “\( A \models \Phi \)” and “\( B \models \Phi \)” are not generally independent, because there exist clauses of length \( k \) that are falsified by both \( A \) and \( B \). On the other hand, qualitatively, as \( k \to \infty \) clausal constraints become progressively “looser”, so that in the limit we can neglect such correlations.

As to the exact expression for \( f_{\infty}(y) \), for a \( k \)-CNF formula the mean-field approximation implies

\[
\Pr[\Phi \in SAT] \sim (1 - c_k^{\gamma_k} n)^{2^n} \sim e^{-2^n \cdot c_k^{\gamma_k} n}.
\]

But since \( c_k \) is specified (in the mean-field approximation) by \( E[\#SAT] \sim 1 \), i.e. \( 2^n \cdot \gamma_k^{c_k n} \sim 1 \), or \( 1 + c_k \log_2 \gamma_k = 0 \), this implies that as \( k \to \infty \)

\[
\Pr[\Phi \in SAT] \sim e^{-2^n [1 - c_k / c_k]} \sim f_{\infty}(y_{\infty,k}).
\]

In other words, when plotted against the annealed order parameters \( y_{ann,k} \) the rescaled satisfaction probability graphs (and their annealed counterparts) punctually converge to the graph of \( f_{\infty} \).

5. Does critical behavior really exist?. The intuitive argument sketched in the preceding paragraph seems to provide a beautiful explanation of the experimental results from [20]. That this intuition is, however, problematic has been shown by Wilson [34]. First note that if the previous argument were true, we would have \( \nu_k = 1 \) for any large enough \( k \), since this is the width of the scaling window that the mean-field versions of \( k \)-SAT predict. On the other hand Wilson presented a simple argument that implies that \( \nu_k \geq 2 \) Hence the above explanation is not rigorously valid.

We stress that Wilson’s observation does not rule out the existence of critical behavior: we, in fact, believe that the qualitative intuition that motivated [20], that versions of \( k \)-SAT become more and more “similar” as \( k \) goes to infinity, is correct. It is the notion of annealed approximation that needs to be changed. And, certainly, his results do not rule the possibility that the rescaled limit probabilities converge, as \( k \to \infty \), to a suitable-defined limit. Obtaining a rigorous example where this holds, that identifies a suitable “annealed approximation that becomes exact” and also obtains an explanation for this convergence, could hopefully offer insights on how to address this problem for random \( k \)-SAT as well. This is what our theorems in the next section provide.

6. Our results. A Horn clause is a disjunction of literals containing at most one positive literal. It will be called positive if it contains a positive literal and negative otherwise. A Horn formula is a conjunction of Horn clauses. Horn satisfiability (denoted by HORN-SAT) is the problem of deciding whether a given Horn formula has a satisfying assignment.

In this chapter we prove a result that displays dimension-dependent behavior for (at most) \( k \)-Horn satisfiability, the natural version of Horn satisfiability studied, parameterized by the
maximum clause length. This problem is also of practical interest in Artificial Intelligence, mainly in connection to theory approximation \cite{18}. The results can be summarized as follows:

1. For an unbounded $k = k(n)$ the threshold phenomenon is essentially the one from the “uniform case” $k(n) = n$. In particular there exists a “rescaled” parameter that makes the graphs of the limit probabilities superimpose (Theorem 6.2).

2. For any constant $k$ the threshold phenomenon is qualitatively described by a suitably chosen queuing model (Theorem 6.4). This yields a closed-form expression for the satisfaction probability when $k = 2$ (Theorem 6.3). This expression has a singularity (though $k = 2$ is likely the only case that does so).

3. The rescaled limit probabilities from the cases when $k$ is a constant converge to the one from the “infinite” case, that can in turn be seen as the result of a mean-field approximation (thus the problem displays what we have called dimension-dependent behavior).

4. Somewhat surprisingly, the explanation for this convergence (an intrinsic feature of the problem) is a threshold property for the number of iterations of PUR (a particular algorithm) on random satisfiable Horn formulas “in the critical range.”

5. In the case when $k = 2$ PUR displays an “easy-hard-easy” pattern for the average number of iterations on satisfiable instances, peaked at the point where the limit probability has a singularity (Theorem 6.6).

Note, however, the important difference between random $k$-SAT and random at-most-$k$-HORN-SAT: for every $k \geq 2$, $k$-SAT has a sharp threshold \cite{9}. All versions of HORN-SAT have coarse thresholds.

**Definition 6.1.** Let $k = k(n) : \mathbb{N} \rightarrow \mathbb{N}$ be monotonically increasing, $1 \leq k(n) \leq n$. We define the following random model $\Omega(k,n,m)$: formula $\Phi$ on $n$ variables is obtained by selecting (uniformly at random and with repetition) $m$ clauses from the set of all (non-empty) Horn clauses in the given variables of length at most $k(n)$.

The following are our results (whose proofs are only sketched):

**Theorem 6.2.** If $k(n) \rightarrow \infty$, $c > 0$, $H_{k(n)}$ is the number of Horn clauses on $n$ variables having length at most $k(n)$, and $m(n) = c \cdot \frac{H_{k(n)}}{n}$ then

$$p_{\infty}(c) := \lim_{n \rightarrow \infty} Pr_{\Phi \in \Omega(k(n),n,m)}(\Phi \in \text{HORN-SAT}) = 1 - F_1(e^{-c}).$$

**Theorem 6.3.** If $c > 0$, and $F_2 : (0,1) \rightarrow (1,\infty)$, $F_2(x) = \ln x / (x - 1)$, then

$$p_2(c) := \lim_{n \rightarrow \infty} Pr_{\Phi \in \Omega(2,n,cn)}(\Phi \in \text{HORN-SAT}) = \begin{cases} 1, & \text{if } c \leq \frac{3}{2}, \\ F_2^{-1}(2c/3), & \text{otherwise}. \end{cases}$$

More generally, define $\lambda_k = \frac{k!}{k+1}$ and $S_j^i = \binom{i}{0} + \binom{i}{1} + \ldots + \binom{i}{j}$ (with the usual convention $\binom{i}{j} = 0$ for $i < j$). Then
THEOREM 6.4. The limit probability $p_k(c) := \lim_{n \to \infty} P_{\Phi \in \Omega(k, n, c \cdot n^{-k-1})}(\Phi \in \text{HORN-SAT})$ is equal to the probability that the following Markov chain ever hits state zero:

$$
\begin{align*}
Q_0 &= 1, \\
Q_{i+1} &= Q_i - 1 + Po(c \cdot \lambda_k \cdot S_{k-2}^{i+1}),
\end{align*}
$$

(6.3)

To get a better intuition on the threshold phenomenon, as displayed by Theorems 6.2, 6.3 and 6.4, we have plotted (in Fig. 1) the limit probability functions $p_2(\cdot), p_3(\cdot), p_\infty(\cdot)$, against the “rescaled” parameter (inspired by Theorem 6.2) $\hat{c} = m \cdot n_{Hk}^m(n)$. This rescaling has the pleasant property that it simplifies the factor $\lambda_k$ from the right-hand side of 6.3, in particular mapping the critical point in Theorem 6.3 to $\hat{c} = 1$. The graphs of $p_2$ (continuous) and $p_\infty$ (dashed) are obtained from their formulas in the previous results, while $p_3$ (dotted) is obtained via simulations. The figure makes apparent that the graphs of $p_2, p_3, \ldots, \ldots$ converge to the graph of $p_\infty$. This statement can be proved rigorously:

THEOREM 6.5. For every $\hat{c} > 0$, $\lim_{n \to \infty} p_n(\hat{c}) = p_\infty(\hat{c})$.

As a bonus our analysis yields the following result:

THEOREM 6.6. Let $q$ be the limit of the expected number of iterations of PUR on a random formula $\Phi \in \Omega(2, n, cn)$, conditional on $\Phi$ being satisfiable. Then

$$
q = \begin{cases} 
\frac{1}{1 - p_2 \lambda_2 c}, & \text{if } c \neq \frac{3}{2}, \\
\infty, & \text{otherwise}.
\end{cases}
$$

(6.4)

This theorem suggests (see Fig.2) and explains the “easy-hard-easy” pattern for the average running time of PUR in this case. Experiments we performed confirm this prediction.
7. Preliminaries. Throughout this paper we use “with high probability” (w.h.p.) as a substitute for “with probability $1 - o(1)$”. We denote (sometimes abusing notation) by $B(n, p)(Po(\lambda))$ a random variable having a binomial (Poisson) distribution with the corresponding parameter(s), and by $\max(a - b, 0)$ the value $\max(a - b, 0)$. We will use the following version of the Chernoff bound

\textbf{Theorem 7.1.} If $0 < \theta < 1/4$ then $\Pr[|B(n, p) - np| > \theta np] \leq e^{-np\frac{\theta^2}{4}}$.

as well as the related inequality from [2]:

\textbf{Proposition 7.2.} Let $P$ have Poisson distribution with mean $\mu$. For $\epsilon > 0$,

$$\Pr[P \leq \mu \cdot (1 - \epsilon)] \leq e^{\epsilon^2 \mu / 2},$$

$$\Pr[P \geq \mu \cdot (1 + \epsilon)] \leq [e^{\epsilon}(1 + \epsilon)^{-(1+\epsilon)}]^{\mu}.$$  

We also use the following inequality:

\textbf{Proposition 7.3.} Let $k \in \mathbb{N}$ and $p \in [0, 1]$. Then for every $n \geq k$

$$1 - \sum_{i=0}^{k-1} \binom{n}{i} p^i (1 - p)^{n-i} \leq \binom{n}{k} p^k.$$  

(7.1)
Proof: Define \( f : [0, 1] \rightarrow \mathbb{R}, f(p) = 1 - \sum_{i=0}^{k-1} \binom{n}{i} p^i (1 - p)^{n-i} - \binom{n}{k} p^k. \) It is easy to see that \( f''(p) = n(n-1)P^{k-1}[(1-p)^{n-k} - 1] \leq 0, \) therefore \( f \) is monotonically decreasing, and \( f(0) = 0. \]

We will also employ couplings of Markov chains (see [33]) to assert stochastic domination. The following is the definition of the type of coupling we employ in this paper:

**Definition 7.4.** Let \((X_t)_t\) and \((Y_t)_t\) be two Markov chains on \(\mathbb{Z}\). A coupling of \(X\) and \(Y\) such that \(X_t \leq Y_t\) is a Markov chain \(Z = (Z_{t,1}, Z_{t,2})\) such that:

- \(Z_{t,1}\) is distributed like \(X_t\) given \(X_0\).
- \(Z_{t,2}\) is distributed like \(Y_t\) given \(Y_0\).
- for every \(i \geq 0\), \(Z_{i,1} \leq Z_{i,2}\).

We use such couplings to bound the probability that a Markov chain \(Y_t\) ever decreases below a certain value \(a\) by coupling it with a chain \(X_t\) such that \(X_t \leq Y_t\) and using the estimate \(\Pr[\exists t : Y_t \leq a] \leq \Pr[\exists t : X_t \leq a]\) that follows from the coupling. The couplings we construct employ the following ideas:

- Suppose the recurrences describing \(\Delta X_t\) and \(\Delta Y_t\) are identical, except for one term, which is \(B(m_1, \tau)\) in \(X_t\) and \(B(m_2, \tau)\) in \(Y_t\), where \(m_1 \geq m_2\) are positive integers and \(\tau \in (0, 1)\). Obtain a coupling by identifying \(B(m_1, \tau)\) with the outcome of the first \(m_1\) Bernoulli experiments in \(B(m_2, \tau)\).
- Suppose now that \(\Delta X_t\) and \(\Delta Y_t\) differ by exactly one term which is \(B(m, p)\) in \(\Delta X_t\) and \(B(m, q)\) in \(\Delta Y_t\), \(p \leq q\). Let \(A_i\) and \(B_i\), \(i = 1, m\), be independent 0/1 experiments with success probabilities \(p\) and \(\frac{q-p}{1-p}\) respectively. Define the pair \((Z_{t,1}, Z_{t,2})\) so that
  1. \(Z_{t,1}\) is the number of times \(A_i\) succeeds.
  2. \(Z_{t,2}\) is the number of times at least one of \(A_i\) and \(B_i\) succeeds.

We measure the distance between two probability distributions \(P\) and \(Q\) by the total variation distance, denoted by \(d_{TV}(P, Q)\), and recall the following results, (see [32] and [3], page 2 and Remark 1.4):

**Lemma 7.5.** If \(n, p, \lambda, \mu > 0\) then \(d_{TV}(B(n, p), \text{Po}(np)) \leq \min\{np^2, \frac{3p}{2}\}\) and \(d_{TV}(\text{Po}(\lambda), \text{Po}(\mu)) \leq |\mu - \lambda|\).

We will also need the following simple lemma:

**Lemma 7.6.** Let \(c\) be a fixed positive integer. For every \(t \in \mathbb{N}\) let \(\xi_t, \eta_t\) be two probability distributions. Define the Markov chains \((X_t)_t\) and \((Y_t)_t\) by recurrences

\[
\begin{align*}
X_{t+1} &= X_t - c + \xi_t, \\
Y_{t+1} &= Y_t - c + \eta_t.
\end{align*}
\]

Then, for every \(t \geq 0\), \(d_{TV}(X_t, Y_t) \leq d_{TV}(X_0, Y_0) + \sum_{i=0}^{t-1} d_{TV}(\xi_i, \eta_i).

**Proof.**

The following result gives a more convenient inequality that immediately implies Lemma 7.6.
LEMMA 7.7. Let \( c \) be a fixed positive integer. Let \( X, Y, \xi, \eta \) be random variables with nonnegative integer values. Define the random variables \( Z \) and \( T \) by recurrences

\[
\begin{align*}
Z &= X - c + \xi, \\
T &= Y - c + \eta.
\end{align*}
\]

Then, for every \( d_{TV}(Z, T) \leq d_{TV}(X, Y) + d_{TV}(\xi, \eta). \)

Proof. 

To prove this result, we will denote (for the “generic” r.v. \( A \)) by \( A_i \) the probability that \( A \) takes value \( i \). We also employ the following simple inequality, valid for \( a, b, c, d \geq 0 \):

\[
|ad - bc| \leq a|d - c| + |a - b|c.
\]

For every \( a \geq 0 \) we have:

\[
\begin{align*}
Z_a &= \sum_{i=0}^{c} X_i \xi_a + \sum_{i=c+1}^{c+a} X_i \xi_{a+1-i}, \\
T_a &= \sum_{i=0}^{c} Y_i \eta_a + \sum_{i=c+1}^{c+a} Y_i \eta_{a+1-i}.
\end{align*}
\]

Applying the above-mentioned inequality and summing we get:

\[
d_{TV}(Z, T) \leq \frac{1}{2} \left\{ \sum_{i=0}^{c} \sum_{a=0}^{\infty} |X_i| \xi_a - \eta_a| + \sum_{i=0}^{c} \sum_{a=0}^{\infty} |X_i - Y_i| \eta_a + \\
+ \sum_{i=c+1}^{c+a} \sum_{a=0}^{\infty} |X_i| \xi_{c+a-i} - \eta_{c+a-i} | + \sum_{i=c+1}^{c+a} \sum_{a=0}^{\infty} |X_i - Y_i| \eta_{c+a-i} \right\}.
\]

Let \( A, B, C, D \) be the four terms of the sum. By simple algebraic manipulations we obtain:

\[
\begin{align*}
A &= \left( \sum_{i=0}^{c} X_i \right) \cdot d_{TV}(\xi, \eta), \\
C &= \left( \sum_{i=c+1}^{c+a} X_i \right) \cdot d_{TV}(\xi, \eta), \\
B &= \frac{1}{2} \sum_{i=0}^{c} |X_i - Y_i|, \\
D &= \frac{1}{2} \sum_{i=c+1}^{c+a} |X_i - Y_i|,
\end{align*}
\]

and the result follows.

Finally, we need the following trivial occupancy property:

LEMMA 7.8. Let \( a \) white balls and \( b \) black balls be thrown uniformly at random in \( n \) bins.

1. if \( r = \max(a, b) = o(n^{1/2}) \) then the probability that there is a bin that contains both white and black balls is at most \( \frac{a^2}{n} = o(1) \).

2. if \( s = \min(a, b) = \omega(n^{1/2}) \) then the probability that there is a bin that contains both white and black balls is \( 1 - o(1/poly) \).

Proof. The first part is easy: the probability that two balls (of any color) end up in the same bin is at most \( \binom{a+b}{2} \cdot \frac{1}{n} \). For the second part, let \( A \) be the event that no two balls of different
colors end up in the same bin, and let $B$ the event that at least $\sqrt{n}$ bins contain white balls. We have:

$$\Pr[A] \leq \Pr[A|B] + \Pr[B].$$

But

$$\Pr[B] \leq \left(\frac{n}{\sqrt{n}}\right)^a \cdot n^{\sqrt{n}-a/2} = o\left(\frac{1}{\text{poly}}\right),$$

and

$$\Pr[A|B] \leq (1 - \frac{1}{\sqrt{n}})^b \sim e^{-b/\sqrt{n}} = o\left(\frac{1}{\text{poly}}\right).$$

The algorithm PUR is displayed in Figure 3. We regard PUR as working in stages, indexed by the number of variables still left unassigned; thus, the stage number decreases as PUR moves on. We say that formula $\Phi$ survives Stage $t$ if PUR on input $\Phi$ does not halt at Stage $t$ or earlier. Let $\Phi_i$ be the formula at the beginning of stage $i$, and let $N_i$ denote the number of its clauses. We will also denote by $P_{i,t}(N_{i,t})$, the number of clauses of $\Phi_i$ of size $i$ and containing one (no) positive literal. Define $\Phi_{i,t}^P (\Phi_{i,t}^N)$ to be the subformula of $\Phi_t$ containing the clauses counted by $P_{i,t}(N_{i,t})$.

The following lemmas were proved in [17], in the context of analyzing the behavior of PUR on $\Phi \in \Omega(n, n, m)$, $m = c \cdot 2^n$.

**Lemma 7.9.**
1. Suppose PUR does not halt before stage $t$. Then, conditional on $N_t$, the clauses of $\Phi_t$ are random and independent.
2. Suppose now that we condition on $\Gamma_t = (N_{1,t}, N_{2,t} P_{1,t}, P_{2,t}$ and on the fact that $\Phi$ survives Stage $t$ as well. Then we have

$$(7.4) \quad N_{t-1} = N_{t} - \Delta_{1,P}(t) - \Delta_{2,P}(t),$$

where

- $\Delta_{1,P}(t)$, the number of positive clauses that are satisfied at stage $t$, has the distribution $1 + B(P_{1,t} - 1, \frac{1}{2})$.
- $\Delta_{2,P}(t)$, the number of positive non-unit clauses that are satisfied at stage $t$, has the binomial distribution $B(P_{2,t}, \frac{1}{2})$.

**Lemma 7.10.** For every $c > 0$ and every $t$, $n-c\sqrt{n} \leq t \leq n$, the conditional probability that the inequality

$$(7.5) \quad N_n - (n-t)\left[1 + \frac{2(N_n - 1)}{t}\right] \leq N_j \leq N_n$$

holds for all $t \leq j \leq n$, in the event that PUR reaches stage $t$, is $1 - o(1)$. 

\[\square\]
Program PUR(Φ):
    if (Φ contains no positive literal as a clause)
      return TRUE
    else
      choose such a positive unit clause x
      if (Φ contains x as a clause)
        return FALSE
      else
        let Φ’ be the formula obtained by setting x to 1
        return PUR(Φ’)

Fig. 7.1. Algorithm PUR

Lemma 7.11. Let Xn ∈ [0, n] be the r.v. denoting the number of iterations of PUR on a random satisfiable formula Φ ∈ Ω(n, c · 2n). Then Xn converges in distribution to a distribution ρ on [0, n] having support on the nonnegative integers, ρ = (ρk)k≥0, ρk = Prob[ρ = k], given by

$$
ρ_k = \frac{e^{-2^k c}}{1 - F(e^{-c})} \prod_{i=1}^{k-1} (1 - e^{-2^i c}).
$$

8. The proof of Theorem 6.2. Let c1 < c2 < c3 be arbitrary constants. Consider three random formulas Φ1 ∈ Ω(n, k(n), c1 · \(\frac{H_k(n)}{n}\)), Φ2 ∈ Ω(n, n, c2 · 2n) and Φ3 ∈ Ω(n, k(n), c3 · \(\frac{H_k(n)}{n}\)), and let Φ’ be the subformula of Φ2 consisting of the clauses of size at most k(n).

By the Chernoff bound, with high probability, m’, the number of clauses of Φ’, is in the interval \([c_1 \cdot \frac{H_k(n)}{n}, c_3 \cdot \frac{H_k(n)}{n}]\). When \(n \to \infty\) the probability that Φ2 ∈ HORN-SAT tends to \(1 - F_1(e^{-c_2})\).

From Lemma 7.11 we infer the following easy consequence

Claim 1. The probability that PUR accepts Φ2 after stage \(n - k(n) + 1\) is o(1).

Since in the first \(k(n) - 1\) stages of PUR only the clauses of Φ’ can influence the algorithm acceptance/rejection of Φ2 (because PUR accepts/rejects at Stage i based only on the unit clauses, and each non-simplified clause loses at most one literal at each phase),

\[|\Pr[Φ_2 \in HORN-SAT] - \Pr[Φ' \in HORN-SAT]| = o(1).\]

By the monotonicity of SAT and the randomness of Φ1, Φ2, Φ’ we have

\[\Pr[Φ_1 \in HORN-SAT] - o(1) \leq \Pr[Φ_2 \in HORN-SAT] \leq \Pr[Φ_3 \in HORN-SAT] + o(1).\]

Taking limits it follows that

\[
\lim_{n \to \infty} \Pr_{Φ \in Ω(n, k(n), c_1 H_k(n)/n)} [Φ \in HORN-SAT] \leq 1 - F(e^{-c_2}) \leq \lim_{n \to \infty} \Pr_{Φ \in Ω(n, k(n), c_3 H_k(n)/n)} [Φ \in HORN-SAT].
\]
Since $c_1, c_2, c_3$ were chosen arbitrarily, by choosing $c_1 = c$, $c_2 = c + \epsilon$, and $c_2 = c - \epsilon$, $c_3 = c$, respectively, we infer that

$$1 - F_1(e^{-(c-\epsilon)}) \leq \lim_{n \to \infty} \Pr_{\Phi \in \Omega(n,k(n),cH_{k(n)}/n)}[\Phi \in \text{HORN-SAT}] \leq \lim_{n \to \infty} \Pr_{\Phi \in \Omega(n,k(n),cH_{k(n)}/n)}[\Phi \in \text{HORN-SAT}] \leq 1 - F_1(e^{-(c+\epsilon)}).$$

As $\epsilon$ is arbitrary, we get the desired result. \qed

**Observation 2.** One point about the previous proof that is intuitively clear, but gets somewhat obscured by the technical details of the proof, is that if $\Phi_2 \in \Omega(n,k(n),c \cdot 2^{n})$ then $\Phi'$ behaves “for every practical purpose” as if it were a uniform formula in $\Omega(n,k(n),c \cdot \frac{H_{k(n)}}{n})$. We will use a similar intuition in the proof of Proposition 9.5.

**9. The uniformity lemma.** The following lemma is the analog of Lemma 7.9 for the case $k = 2$, and the basis for our analysis of this case:

**Lemma 9.1.** Suppose that $\Phi$ survives up to stage $t$. Then, conditional on $(P_{1,t}, N_{1,t}, P_{2,t}, N_{2,t})$, the clauses in $\Phi_{1,t}, \Phi_{1,t}, \Phi_{2,t}, \Phi_{2,t}$ are chosen uniformly at random and are independent. Also, conditional on the fact that $\Phi$ survives stage $t$ as well, the following recurrences hold:

$$\begin{align*}
P_{1,t-1} &= P_{1,t} - 1 - \Delta_{1,t}^P + \Delta_{12,t}^P, \\
N_{1,t-1} &= N_{1,t} + \Delta_{12,t}^N, \\
P_{2,t-1} &= P_{2,t} - \Delta_{12,t}^P - \Delta_{02,t}^P, \\
N_{2,t-1} &= N_{2,t} - \Delta_{12,t}^N, \\
\end{align*}$$

(9.1)

where (in distribution)

$$\begin{align*}
\Delta_{1,t}^P &= B(P_{1,t} - 1, 1/t), \\
\Delta_{12,t}^P &= B(P_{2,t}, 1/t), \\
\Delta_{02,t}^P &= B(P_{2,t} - \Delta_{12,t}^P, 1/t), \\
\Delta_{12,t}^N &= B(N_{2,t}, 2/t).
\end{align*}$$

(9.2)

**Proof.** A formula will be represented by an $m \times 2$ table. The rows of the table correspond to clauses in the formula and the entries are its literals. They are gradually unveiled as the algorithm proceeds. We assume that when generating $\Phi$ we mark those clauses containing only one literal (so that we know their location, but not their content). We say that a row (or a clause) is “blocked” either if the clause is already satisfied or the clause has been turned into the empty clause. Suppose PUR arrives at stage $t$ on $\Phi$. Then in stages $i = n, n - 1, \ldots, t + 1$, $\Phi_i$ should contain a unit clause consisting of a positive literal but should not have contained complementary unit clauses of the same variable. To carry out the disclosure at stage $i$, let $x$ be the variable set to one in this stage. We assume that the formula unveils all occurrences of $x$ or $\overline{x}$ in $\Phi$. For each clause we perform the following:

1. if it contains $x$ we unveil all its literals and block;
2. otherwise we do nothing.
The clauses of $\Phi_t$ having size two correspond to the rows of $\Phi$ that contain no unveiled literal. The clauses of size one are either the clauses of size one in $\Phi$ that contain none of the chosen literals, or the clauses of size two that contain the negation of one chosen variable and another is yet to be chosen. Given these observations the uniformity and independence follow from the way we construct $\Phi$.

To prove the recurrences, let $x$ be the variable set to one in stage $t$ (it exists since PUR does not halt at this stage). By uniformity and independence, each of the $P_{1,t} - 1$ positive unit clauses of $\Phi_t$, other than the chosen one, is equal to $x$ with probability $1/t$ (since there are $t$ variables left at this stage). On the other hand, the positive unit clauses of $\Phi_{t-1}$ that are not present in $\Phi_t$ can only come from clauses of size two of $\Phi_t$ that contain $x$ and a positive literal (therefore counted by $P_{2,t}$). Uniformity and independence imply therefore that $\Delta^P_t(t)$ has the distribution claimed in (9.2). The other relations can be justified similarly (noting that, since PUR does not reject at this stage, every negative unit clause of $\Phi_t$ is also present in $\Phi_{t-1}$).

It will be useful to consider the Markov chain (9.1) for all values of $t = n, \ldots, 0$ (even when the algorithm halts). To accomplish that, the “minus” signs in the first equation of (9.1) and the definition of $\Delta^P_t$ should be replaced by $\dot{=}$ . We also need to specify the distribution of each component of the tuple $(P_{1,n}, N_{1,n}, P_{2,n}, N_{2,n})$. Let $\Delta_n$ be a random variable having the Bernoulli distribution $B(cn, 2n/(2n+3(\sqrt{2})^2))$. It is easy to see that in distribution

$$
\begin{align*}
P_{1,n} &= B(\Delta_n, 1/2), \\
N_{1,n} &= \Delta_n - P_{1,n}, \\
P_{2,n} &= B(cn - \Delta_n, 2/3) \\
N_{2,n} &= cn - \Delta_n - P_{2,n}.
\end{align*}
$$

(9.3)

10. Proof of Theorem 6.3. The main intuition for the proof is that in “most interesting stages” $\Delta^P_t = 0$ and $\Delta^P_{12,t}$ is approximately Poisson distributed. Therefore, $P_{1,t}$ qualitatively behaves like the Markov Chain $(Q_t)_t$ defined by

$$
\begin{align*}
Q_{n+1} &= 1, \\
Q_{t-1} &= Q_{t-1} + Po(\lambda),
\end{align*}
$$

(10.1)

where $\lambda = 2c/3$. This explains the closed form of the limit probability: a well-known result states that $\rho$, the probability that the queuing chain $Q_t$ reaches state 0, satisfies the equation $\rho = \Phi(\rho)$, where $\Phi(t) = e^{\lambda(t-1)}$ is the generating function of the arrival distribution $Po(\lambda)$.

We will define a suitable value $\omega_0$ such that:

1. With high probability PUR does not reject in any of stages $n, \ldots, n - \omega_0$.
2. PUR accepts “mostly before or at stage $n - \omega_0$” (i.e. the probability that PUR accepts after stage $n - \omega_0$, given that $\Phi$ survives this far is $o(1)$).
3. With high probability, for every $t \in n, \ldots, n - \omega_0$, $\Delta^P_t = 0$.
4. At stages $n, \ldots, n - \omega_0$, $P_{1,t}$ is “very close” to $Q_t$, with respect to total variation distance.

This program can be accomplished as described if $c < 3/2$. To prove Property 4 we make use of Lemmas 7.5 and 7.8. Property 2 is proved only implicitly: in this case (see [15]) the probability that $Q_t = 0$ for some $i$ tends to one, and, in fact, by a technical result due to Frieze and Suen (Lemma 3.1 in [10]), $Pr[Q_i = 0$ for some $i \geq n - \log n] = 1 - o(1)$.
Let us now concentrate on the case when \( c > 3/2 \) (the case when \( c = 3/2 \) will follow by a monotonicity argument). In the previous argument we only used the fact that \( c < 3/2 \) when deriving the probability that \( Q_1 \) hits state 0, hence the arguments from above carry on, and the conclusion is that the probability that PUR accepts at one of the stages \( n, \ldots, n - \omega_0 \) differs by \( o(1) \) from the probability that \( Q_1 = 0 \) somewhere in this range. We now, however, have to consider the probability that PUR accepts at some stage later than \( n - \omega_0 \) and aim to prove that this probability is \( o(1) \). It is conceptually simpler to divide the interval \([n - \omega_0, n]\) into two subintervals, \([n - \omega_0, n - \omega_1]\) and its complement, such that w.h.p. \( \Phi_{n - \omega_1} \) (if defined) contains two opposite unit clauses, therefore the probability that PUR accepts after stage \( n - \omega_1 \) is \( o(1) \). In the range \([n - \omega_0, n - \omega_1]\) we would like to prove that “most of the time” \( \Delta^P_{1,t} \) is zero and \( P_{1,t} \) is “close” to \( Q_t \) and to reduce the problem to the analysis of \( Q_t \). Unfortunately there are two problems with this approach: although the probability that each individual \( \Delta^P_{1,t} > 0 \) is fairly small, to make \( \Phi_{n - \omega_1} \) unsatisfiable w.h.p., \( \omega_1 \) has to be \( \omega(\sqrt{n}) \). This implies that we cannot sum these probabilities over \([n - \omega_0, n - \omega_1]\) and expect the sum to be \( o(1) \); a similar problem arises if we want to sum the upper bounds for \( d_{TV}(\Delta^P_{12,t}, \Phi_{n - \omega_0}) \).

Fortunately there is a way to circumvent this, avoiding the use of total variation distance altogether: although we cannot guarantee that w.h.p. each \( \Delta^P_{1,t} = 0 \), we can arrange that w.h.p. for every sequence of \( p \) consecutive stages \( t, t - 1, \ldots, t - p + 1, \Delta^P_{1,t} + \Delta^P_{1,t-1} + \ldots + \Delta^P_{1,t-p+1} \leq 3(\ast) \). Intuitively, in any sequence of \( p \) consecutive steps at most \( p + 3 \) clients leave the queue, and the number of those who arrive is the sum of \( p \) approximately Poisson variables, thus approximately Poisson with parameter \( p \lambda \). Choosing \( p \) large enough so that \( \lambda > 1 + \frac{2}{p} \) ensures that in any \( p \) steps the average number of customers that arrive is strictly larger than the number of customers that are served in this time span. Therefore we will seek to approximate \( P_{1,t} \) by a queuing chain \( \mathcal{Q}_t \) with this property. Since \( P_{1,n - \omega_0} = \mathcal{Q}_t \) is “large,” an elementary analysis of the queuing chain implies that the probability that \( \mathcal{Q}_t \) hits state 0 in the interval \([n - \omega_0, n - \omega_1]\) is exponentially small. So we obtain the desired result if \( \mathcal{Q}_t \) is constructed so that it is stochastically dominated by \( P_{1,t} \).

10.1. The case \( c < 3/2 \). Define \( \omega_0 = n^{0.1} \). The following are the main steps of the proof in this case:

**Lemma 10.1.** With probability \( 1 - o(1/poly) \) for every \( t \in [n, \ldots, n/2] \) we have

\[
\Delta^P_{12,t}, \Delta^P_{02,t}, \Delta^N_{12,t} \leq \frac{1}{2} n^{0.1}.
\]

**Proof.** Use the coupling with \( m_1 = P_{2,t}(\mathbf{N}_{2,t}), m_2 = cn, \tau = 1/t \), and apply Chernoff bound to \( B(cn, 1/t) \).

**Corollary 1.** Consider \( \omega \leq n/2 \). If for every \( t \in [n, \ldots, n/2] \), \( \Delta^P_{12,t}, \Delta^P_{02,t}, \Delta^N_{12,t} \leq \frac{1}{2} n^{0.1} \) then, for all \( t \in [n, \ldots, n - \omega] \), \( P_{1,t}, N_{1,t}, |P_{2,t} - P_{2,n}|, |N_{2,t} - N_{2,n}| < (n-t) \cdot n^{0.1} \).

**Lemma 10.2.** If for all \( t \in [n, \ldots, n - \omega] \), \( P_{1,t}, N_{1,t}, |P_{2,t} - P_{2,n}|, |N_{2,t} - N_{2,n}| < (n-t) \cdot n^{0.1} \) holds then w.h.p. \( \Delta^P_{1,t} = 0 \) for every \( t \in [n, \ldots, n - \omega_0] \).
Proof. \( \Pr[B(P_{1,t} - 1, \frac{1}{t}) > 0] = 1 - \Pr[B(P_{1,t} - 1, \frac{1}{t}) = 0] = 1 - (1 - \frac{1}{t}) P_{1,t}^{-1} < \frac{P_{1,t}^{-1}}{t} < n^{-0.9} \). □

Lemma 10.3. W.h.p., \(|P_{2,n} - \frac{2}{3}cn|, |N_{2,n} - \frac{1}{6}cn| < n^{0.6}\).  
Proof. Directly from the Chernoff bounds on \( \Delta_n \) and \( P_{2,n} \). □

Lemma 10.4. If the events in the conclusions of Lemmas 1 and 10.3 hold for \( \omega = \omega_0, \epsilon_1 = 1/6 \) and \( \epsilon_2 = 0.1 \), then there exists a constant \( r > 0 \) such that for every \( t = n, \ldots, n - \omega_0 \), \( |P_{2,t} - \frac{2}{3}c| \leq rn^{-0.4} \).

Proof. We have
\[
|P_{2,t} - \frac{2}{3}c| \leq P_{2,t} \left| \frac{1}{t} - \frac{1}{n} \right| + \frac{|P_{2,t} - P_{2,n}|}{n} \leq \frac{P_{2,n}}{n} \left( \frac{\omega_0}{n(n - \omega_0)} \right) + \frac{n^{0.2}}{n} + n^{0.6-1},
\]
by Lemma 10.4 and \( n - \omega_0 \leq t \leq n \), and the result immediately follows. □

Lemma 10.5. If the conclusions of Lemmas 10.4 and 10.2 are true then
\[
\sum_{t=n-\omega_0}^{n} d_{TV}(P_{1,t}, Q_t) = o(1/\omega_0).
\]

Proof. By Lemma 10.4 and the inequalities on total variation distance there exist \( r_1, r_2 > 0 \) such that
\[
d_{TV}(\Delta_{12,t}^P, Po(\lambda)) \leq d_{TV} \left( \Delta_{12,t}^P, Po \left( \frac{P_{2,t}}{t} \right) \right) + d_{TV} \left( Po \left( \frac{P_{2,t}}{t} \right), Po \left( \frac{2}{3}c \right) \right) \leq r_1 \frac{1}{t} + r_2 n^{-0.4} \leq r_3 n^{-0.4},
\]
where \( r_3 = r_1 + r_2 \). Employing Lemma 7.6 it follows that
\[
\sum_{t=n-\omega_0}^{n} d_{TV}(P_{1,t}, Q_t) \leq r_3 \sum_{t=n-\omega_0}^{n} tn^{-0.4} \leq r_3 n^{-0.4} \frac{\omega_0^2}{2},
\]
and this amount is \( o(1/\omega_0) \). □

Observation 3. The probability that the conditions in the previous lemma are not fulfilled is at most \( \omega_0^A/n = n^{-0.6} \). Indeed, the events that ensure the applicability of the previous lemma are:
Therefore the probability that for some \( \omega \), \( \Delta_{12,t}^P, \Delta_{02,t}^P, \Delta_{12,t}^N \leq \frac{1}{2}n^{0.1} \),

2. for all \( t \in [n, n - \omega_0] \), \( \Delta_{i,t}^P = 0 \), and

3. \( |P_{2,n} - \frac{2}{n}cn|, |N_{2,n} - \frac{1}{3}cn| < n^{0.6} \)

The first and the third events have probability \( 1 - o(1/\text{poly}) \) (as they come from applying Chernoff bounds). The second fails (for a specific \( t \)) with probability at most \( \frac{P_{1,n}}{n} \leq \omega_0^2/(n - \omega_0) \), so its total probability is at most \( \omega_0 \cdot \omega_0^2/(n - \omega_0) \). Both terms can be absorbed into \( \omega_0^4/n \).

**Lemma 10.6.** If the event in Lemma 7 holds then w.h.p. PUR does not reject at stage \( t \), for every \( t \) in the range \( n, n - 1, \ldots, n - \omega_0 \), given that \( \Phi \) survives up to this stage.

**Proof.** To prove Lemma 10.6 we show that, with high probability the unit clauses of each \( \Phi_t \) involve different variables. This can be seen as follows: consider \( P_{1,t} + N_{1,t} \) balls to be thrown into \( t \) urns. The probability that two of them arrive in the same urn is at most \( (P_{1,t} + N_{1,t}) \cdot \frac{1}{t} \). This is upper bounded by \( \frac{\omega_0^{n+1}}{2(n - \omega_0)^2} \). Summing this for \( t = n, \ldots, n - \omega_0 \) yields an upper bound, which is \( o(1) \).

The proof for the case \( c < 3/2 \) follows easily from these results: with probability \( 1 - o(1) \) all the events in Lemmas 10.1, 10.2, 10.3, 10.5 and 10.6 take place, therefore PUR does not reject at any of the stages \( n \) to \( n - \omega_0 \) and \( P_{1,t} \) is close to \( Q_t \) in the sense of Lemma 10.5. Therefore the probability that for some \( t \) in this range \( P_{1,t} = 0 \) (i.e. PUR accepts) differs by \( o(1) \) from the corresponding probability for \( Q_t \). But according to the result by Frieze and Suen 10, this latter probability is \( 1 - o(1) \).

10.2. The case \( c > 3/2 \). Define \( \omega_1 = n^{0.51} \). The following are the auxiliary results we use in this case:

**Lemma 10.7.** Let \( A = n^{0.61} \). For every \( k > 0 \) there exists a constant \( c_k > 0 \) such that for every \( r > 0 \) the probability that there exists \( t \in [n - \omega_0, n - \omega_1] \), \( \Delta_{i,t}^P + \Delta_{i,t-1}^P + \ldots + \Delta_{i,t-r+1}^P \geq k \) is at most \( c_k(\omega_1 - \omega_0)(rA/n)^k \).

**Proof.** By Corollary 1 we can assume that \( P_{1,t} \leq A \). Then for every \( i \),

\[
Pr[\Delta_{i,t}^P \geq i] = Pr[B(P_{1,t} - 1, 1/t) \geq i] \leq Pr[B(A, 1/t) \geq i]
\]

\[
= 1 - \sum_{j=1}^{i-1} \binom{A}{j} \left(1 - \frac{1}{t}\right)^j \frac{1}{t}^{A-j}
\]

\[
\leq \binom{A}{i} \left(\frac{1}{t}\right)^i
\]

The event \( \Delta_{i,t}^P + \Delta_{i,t-1}^P + \ldots + \Delta_{i,t-r+1}^P \geq k \) happens when:

* one of the factors is at least \( k \), or
* one of the factors is at least \( k - 1 \), and another one is at least 1, or
of the queuing chain, the probability that (11.1)

\[ P \]

definition of the chain \( \alpha \)

22

G. ISTRATE

will be slightly nonstandard (to reflect the connection with the indices starts with \( \omega \) and is decreasing.

To flesh out the argument outlined before we construct a succession of Markov chains running along \( P_{1,t} \), that provide better and better “approximations” to \( Q_t \). Our use of indices will be slightly nonstandard (to reflect the connection with \( P_{1,t} \)), in that the sequence of indices starts with \( n - \omega \) and is decreasing.

**Definition 10.8.** Let \( X_{n-\omega} = Y_{n-\omega} = Z_{n-\omega} = Q_{n-\omega} = P_{1,n-\omega} \) and

\[
\begin{align*}
X_{t-1} &= X_t - (p + 3)\chi_{\omega}Z_{t+1}(n - \omega_0 - t) + \Delta_{12,t}^P, \\
Y_{t-1} &= Y_t - (p + 3)\chi_{\omega}Z_{t+1}(n - \omega_0 - t) + B(P_{2,n-\omega}, 1/t), \\
Z_{t-1} &= Z_t - (p + 3)\chi_{\omega}Z_{t+1}(n - \omega_0 - t) + B(P_{2,n-\omega}, \frac{1}{n}), \\
Q_{t-1} &= Q_{t-1} - 1 + B(p(\frac{P_{2,n-\omega}}{p+3}), \frac{1}{n}).
\end{align*}
\]

Let \( c = \Pr[\exists t \in [n - \omega_0, n - \omega_1]) : P_{1,t} = 0] \). Note that the amount \( p + 3 \) is subtracted from \( X_t, Y_t, Z_t \) exactly once in every \( p \) consecutive steps, so whenever the condition (*) is satisfied it holds that \( X_t \leq P_{1,t} \) for every \( t \in [n - \omega_0, n - \omega_1] \). By coupling \( \Delta_{12,t}^P(= B(P_{2,t}, 1/t)) \) with \( B(P_{2,n-\omega}, 1/t) \) we deduce that we can couple \( X_t \) and \( Y_t \) so that \( Y_t \leq X_t \). We can also couple \( Y_t \) and \( Z_t \) such that \( Z_t \leq Y_t \). Finally, notice that we can couple \( Z_{n-\omega_0-jp} \) and \( Q_{n-\omega_0-jp} \) such that \( Q_{n-\omega_0-jp} \leq Z_{n-\omega_0-jp} \). So an upper bound on \( \alpha \) is \( \Pr[\exists t \in [0, n - \omega_0]) : Q_t = 0] \). With high probability the Bernoulli distribution in the definition of the chain \( Q_t \) has the average strictly greater than one, (because the flow from \( P_{2,t} \) is approximately Poisson), and \( Q_{n-\omega_0} = \Omega(\omega_0) \), therefore, by an elementary property of the queuing chain, the probability that \( Q_t \) hits state 0 is exponentially small. This yields the desired conclusion, that \( \alpha = o(1) \).

One word about the way to prove the fact that \( \Phi_{n,\omega_1} \) is unsatisfiable (if defined): one can prove that w.h.p. both \( P_{1,n-\omega_1} \) and \( N_{1,n-\omega_1} \) are \( \Omega(\omega_1) \). By the uniformity lemma 7.3 we are left with the following instance of the occupancy problem: there are \( P_{1,n-\omega_1} \) white balls, \( N_{1,n-\omega_1} \) black balls and \( n - \omega_1 \) bins. The desired fact now follows from the second part of Lemma 7.3.

**11. Proof of Theorem 6.4** Theorem 6.4 is proved along lines very similar to the proof of Theorem 6.3. The basis is the following generalization of Lemma 9.1.

**Lemma 11.1.** Suppose that \( \Phi \) survives up to stage \( t \). Then, conditional on the values \( (P_{1,t}, N_{1,t}, \ldots, P_{k,t}, N_{k,t}) \), the clauses in \( \Phi_{1,t}^P, \Phi_{1,t}^N, \ldots, \Phi_{k,t}^P, \Phi_{k,t}^N \) are chosen uniformly at random and are independent. Also, conditional on the fact that \( \Phi \) survives stage \( t \) as well, the following recurrences hold:

\[
\begin{align*}
P_{1,t-1} &= P_{1,t} - 1 - \Delta_{01,t}^P + \Delta_{12,t}^P, \\
N_{1,t-1} &= N_{1,t} + \Delta_{12,t}, \\
P_{i,t-1} &= P_{i,t} - \Delta_{0i,t}^P - \Delta_{(i-1)i,t}^P + \Delta_{(i+1)i,t}^P, \text{ for } i = 2, k, \\
N_{i,t-1} &= N_{i,t} - \Delta_{(i-1)i,t}^N + \Delta_{(i+1)i,t}^N, \text{ for } i = 2, k.
\end{align*}
\]
where (in distribution)

\[
\begin{align*}
\Delta_{0,i,t}^P &= B(P_{1,t} - 1, 1/t), \\
\Delta_{(i-1),t}^P &= B(P_{i,t}, (i - 1)/t), \\
\Delta_{0,i,t}^N &= B(P_{i,t}, (i - 1)/t, 1/t), \\
\Delta_{(i-1),t}^N &= B(N_{i,t}, i/t), \\
\Delta_{k(k+1),t}^N &= \Delta_{k(k+1),t}^N = 0.
\end{align*}
\]

(11.2)

Proof.

The uniformity condition and the justification of the recurrences are absolutely similar to the ones from Lemma 6.3. The additional technical complication is that now there is a “positive flow into $P_{2,t}, N_{2,t}$.”

\[ \square \]

Lemma 11.2. With high probability it holds that

\[ P_{i,t} = (1 + o(1)) \cdot \frac{c}{n} \cdot \lambda_k \cdot \binom{t}{i} \cdot S_{k-i}^{n+1-t}, \]

and

\[ N_{i,t} = (1 + o(1)) \cdot \frac{c}{n} \cdot \lambda_k \cdot \binom{t}{i} \cdot S_{k-i}^{n+1-t}, \]

for every $i \geq 2$, and uniformly on $t = n - o(n)$.

Proof.

Let us first heuristically derive a formula for $x_{i,t}$, $y_{i,t}$, the expected values of $P_{i,t}$, $N_{i,t}$, obtained by replacing the binomial distributions in the equations by their expected values.

We have:

\[
\begin{align*}
x_{i,t-1} &= x_{i,t} - x_{i,t} \frac{x_{i,t}}{t} + \frac{(i-1)x_{i,t}}{t}, \text{ for } i = \frac{2}{k}, \\
y_{i,t-1} &= y_{i,t} - y_{i,t} \frac{y_{i,t}}{t} + \frac{(i+1)y_{i,t}}{t}, \text{ for } i = \frac{2}{k}.
\end{align*}
\]

Rearranging terms the recurrences become

\[
\begin{align*}
x_{i,t-1} &= x_{i,t} (1 - \frac{i}{t}) + x_{i+1,t} \frac{i}{t}, \text{ for } i = \frac{2}{k}, \\
y_{i,t-1} &= y_{i,t} (1 - \frac{i}{t}) + y_{i+1,t} \frac{i+1}{t}, \text{ for } i = \frac{2}{k}.
\end{align*}
\]

(11.3)

Also,

\[
\begin{align*}
x_{i,n} &= \frac{n!}{H_k} \cdot c \lambda_k \cdot H_{n-k} = \frac{c}{n} \lambda_k \cdot \binom{n}{i}, \\
y_{i,n} &= \frac{n!}{H_k} \cdot c \lambda_k \cdot \frac{H_{n-k}}{n} = \frac{c}{n} \lambda_k \cdot \binom{n}{i}.
\end{align*}
\]

A simple induction shows that these expected values are $x_{i,t} = \frac{c}{n} \lambda_k \cdot \binom{t}{i} \cdot S_{k-i}^{n+1-t}$, and $y_{i,t} = \frac{c}{n} \lambda_k \cdot \binom{t}{i} \cdot S_{k-i}^{n+1-t}$.

The concentration property can be proved inductively, starting from $i = k$ towards $3$, by noting that the expected values of the binomial terms in the recurrence are $\omega(n)$, hence,
by the Chernoff bound, the probabilities that they significantly deviate from their expected values is exponentially small.

Almost the same argument holds for \( P_{2,t} \) and for \( N_{2,t} \). The only amounts to be handled differently are “the clause flows out of \( P_{2,t}, N_{2,t} \),” but they are approximately Poisson distributed, hence “small” with high probability by Proposition 7.2. Therefore

\[
P_{2,t} = (1 + o(1)) \frac{c}{n} \cdot \lambda_k \cdot 2^{\left(\frac{t}{2}\right)} \cdot S_{k-2}^{n+1-t}.
\]

The previous lemma implies that \( \Delta P_{2,t} \sim Po\left(\frac{c}{n} \cdot \lambda_k \cdot S_{k-2}^{n+1-t}\right) \) (for \( t = n - o(n) \)); thus in this range \( P_{1,t-1} \sim P_{1,t} - 1 + Po\left(\frac{c}{n} \cdot \lambda_k \cdot S_{k-2}^{n+1-t}\right) \). The proof follows exactly the same pattern as in the case \( c < 3/2 \) for \( k = 2 \): the conclusion for the stages \([n, n - \omega_0]\) is that the probability that \( P_{1,t} \) is zero somewhere in this range differs by \( o(1) \) from the corresponding probability for the queuing chain in (6.3). The fact that the stages after \([n, n - \omega_0]\) have a contribution of \( o(1) \) to the final accepting probability can be seen by the fact that there is possible to couple the Markov \( M_1 \), describing the evolution of PUR on a random \( k \)-SAT formula, and \( M_2 \) that runs on the 2-CNF component of the formula, such that for every \( t \) we have \( P_{M_1}^{M_2} \leq P_{M_1}^{M_2} \). Perhaps the most intuitive way to see this coupling is to “paint” the initial clauses of the formula having size at most two in red, and the other clauses in blue. At every step \( t P_{M_1}^{M_2} \) will count only red clauses having unit size at step \( t \), while \( P_{M_1}^{M_2} \) will count clauses of both colors.

Given the stochastic domination, the desired result follows from the corresponding proof in the case \( k = 2 \).

12. Proof of Proposition 6.5. The idea of the proof is to consider PUR on a random at-most-\( k \)-Horn formula \( \Phi \) with \( \hat{c} \cdot H_k \) clauses and prove that there exists a function \( \phi(k) \) with \( \lim_{k \to \infty} \phi(k) = 0 \) such that

\[
\lim_{n \to \infty} \Pr[\text{PUR accepts in at least } k \text{ steps}] \leq \phi(k).
\]

Indeed, from the previous proof it follows that \( \lim_{n \to \infty} \Pr[\text{PUR accepts in } \geq k \text{ steps}] \) satisfies the recurrence:

\[
x_{t+1} = x_{1,t} - 1 + Po \left(\frac{\hat{c}}{n} \cdot S_{k-2}^{t+1+k}\right),
\]

where

\[
x_0 = P_{1,k} \geq 1.
\]

We define \( \phi(k) \) to be the probability that the sequence in the recurrence (12) hits zero. Trivially \( \lim_{k \to \infty} S_{k}^{n+1} = \infty \), so the expected values of the Poisson distributions in (12) can be made larger than any given constant \( \lambda \). Using the fact that the sum of two Poisson distributions with parameters \( a \) and \( b \) has a Poisson distribution with parameter \( a + b \) it follows that, for large enough \( k \), one can couple \( x_t \) with the queuing chain

\[
y_{t+1} = y_{1,t} - 1 + Po(\lambda),
\]

\[
y_0 = 1,
\]
such that $y_t \leq x_t$. It follows that, for large $k$, $\phi(k) \leq \Pr[\text{the chain } y_t \text{ hits state zero}].$ Since $\lambda$ was arbitrary, it follows that $\lim_{k \to \infty} \phi(k) = 0.$

Now consider a random uniform Horn formula $\Phi$ with $c \cdot \frac{H}{n}$ clauses, and let $\Phi$ be its subformula consisting of clauses of size at most $k$. It is easily seen that the behavior of PUR on the first $k - 1$ steps depends only on the clauses of $\Phi$, so

$$\Pr[\text{PUR accepts } \Phi \text{ in less than } k \text{ steps}] = \Pr[\text{PUR accepts } \Phi \text{ in less than } k \text{ steps}].$$

On the other hand we have

$$0 \leq \Pr[\text{PUR accepts } \Phi \text{ in at least } k \text{ steps}] \leq \Pr[\text{PUR accepts } \Phi \text{ in at least } k \text{ steps}].$$

The fact that “$\Phi$ is close to a random formula in $\Omega(n, k, c \cdot \frac{H}{n})$” (see the discussion in Observation 2) implies that the right-hand side term can be made less than any fixed constant $\epsilon$ (for $n, k$ big enough). It follows that

$$|\Pr[\text{PUR accepts } \Phi] - \Pr[\text{PUR accepts } \Phi]| \leq 2 \cdot \epsilon,$$

for large enough values of $n, k$. This immediately implies the desired result. \qed

13. Proof of Theorem 6.6. Theorem 6.6 is based on the proof of the Theorem 6.3 and an elementary property of the queuing chain $Q_t$ (the expected time to hit state zero, conditional on actually hitting it has the desired form).

The crucial point is to prove that the probabilities that any of the conditions we have employed in our analysis fails have a negligible effect on the running time.

This is easy to see for stages smaller than $n - \omega_0$: since the probabilities that the various steps of the analysis are either exponentially small or can be made $o(1/n)$ (by choosing a large enough $k$ in Lemma 10.7, the probability that $P_{1,t}$ hits state zero after stage $n - \omega_0$ is $o(1/n)$, therefore its influence on the average running time of PUR is $o(1)$. The corresponding observation is not true for stages before $n - \omega_0$, but these stages can be handled directly, using the statement from Lemma 10.5. \qed

14. Random Horn satisfiability as a mean-field approximation. What we have shown so far is to prove that (under a suitably rescaled picture) the rescaled probability graphs for random at-most-$k$ Horn satisfiability converge to the graph for random Horn satisfiability. To be able to argue that our results display critical behavior, we have to be able to show that this latter probability $p_{\infty}$ is indeed the one predicted by some mean-field approximation.

In the sequel we will show that this is indeed the case. However the mean-field approximation is not the one from [20], and incorporates a correction specific to the properties of random Horn satisfiability.

Let us first see that it is not accurate if no correction is taken into account. Indeed, were it true we would have

$$\lim_{n \to \infty} \Pr[\Phi \in \text{HORN-SAT}] = 1 - \lim_{n \to \infty} \prod_{A \in \{0,1\}^n} (1 - \Pr[A \models \Phi]).$$

Since, for an assignment $A$ of Hamming weight $i$ there are exactly $2^i - 1 + (n - i) \cdot 2^i$ Horn clauses that $A$ falsifies, we have
Pr[A |= Φ] = \left(1 - \frac{2^i - 1 + (n - i) \cdot 2^j}{(n + 2) \cdot 2^n - 1}\right)^{c \cdot 2^n},

so the mean-field prediction reads

\lim_{n \to \infty} \Pr[Φ ∈ HORN-SAT] = 1 - \lim_{n \to \infty} \prod_{j=0}^{n} \left(1 - \frac{2^j - 1 + (n - j) \cdot 2^j}{(n + 2) \cdot 2^n - 1}\right)^{c \cdot 2^n}.

All terms in the product are less than 1. Since the term corresponding to \( j = 1 \) is \( \left(1 - \frac{2^j - 1 + (n - j) \cdot 2^j}{(n + 2) \cdot 2^n - 1}\right)^n \) has limit 0, the mean-field prediction would imply that

\lim_{n \to \infty} \Pr[Φ ∈ HORN-SAT] = 1. \quad \text{(5)}

On the other hand let us observe that, if we do not consider the power \( (n) \) in the infinite product we obtain the right result: it is a simple but tedious task to prove that

\lim_{n \to \infty} \prod_{j=0}^{n} \left(1 - \frac{2^j - 1 + (n - j) \cdot 2^j}{(n + 2) \cdot 2^n - 1}\right) = \prod_{j=0}^{\infty} \left(1 - e^{-c \cdot 2^j}\right).

Intuitively this means that “there exist a correction of the mean-field approximation that only considers a single assignment of each weight, and is accurate.” The following simple result gives a precise statement to the above intuition:

**Lemma 14.1.** Suppose Φ is given as a union of formulas Φ_1, . . . , Φ_n, where Φ_i contains all clauses of length exactly i. Then there is a set \( T = \{T_0, \ldots, T_{n-1}\} \) of assignments, with \( T_i \) of Hamming weight exactly i and depending only on \( Φ_1 \cup \ldots \cup Φ_{i+1} \), such that Φ is satisfiable if and only if it is satisfied by some assignment in \( T \).

**Proof.**

Let \( y_1 \ldots y_k \) denote the assignment that makes \( y_1 = \ldots = y_k = 1 \), and all the other variables equal to zero.

The set \( T \) has two parts: the first is simply the set of assignments implicitly examined by the algorithm PUR in testing satisfiability. That is, if \( x_1, \ldots, x_k \) are the variables assigned by PUR in this order, the first part includes the assignments 00000, \( \overline{x_1}, \ldots, \overline{x_1}, \ldots, x_k \). The second part contains a random assignment for each remaining weight. \( \square \)

The result has a “mean-field” interpretation: as before, define \( f(x_1, \ldots, x_n) = 1 - \prod_{i=1}^{n} x_i \), and the function \( g_k[Φ] \) to be the indicator function for the event “\( T_k \not|= Φ \), given that event \( \overline{A_n} \land \ldots \land \overline{A_{n-k+1}} \) happens,” i.e.

\[ g_k[Φ] = \frac{1}{Pr[A_n \land \ldots \land \overline{A_{n-k+1}}]} \cdot \begin{cases} 1, & \text{if } T_k \not|= Φ \land \overline{A_n} \land \ldots \land \overline{A_{n-k+1}} \\ 0, & \text{otherwise.} \end{cases} \]

We have

\[ E[g_k[Φ]] = Pr[A_{n-k} | A_n \land \ldots \land \overline{A_{n-k+1}}]. \]

Indeed, \( g_k[Φ] \neq 0 \) exactly when \( R_n \lor \ldots \lor R_{n-k+1} \) or \( T_k \not|= Φ \land S_n \land \ldots S_{n-k+1} \). The second event is equivalent to \( \overline{A_{n-k}} \land S_n \land \ldots S_{n-k+1} \), hence we have \( g_k[Φ] \neq 0 \) exactly when \( \overline{A_{n-k}} \land \overline{A_n} \land \ldots \land \overline{A_{n-k+1}} \) holds.
Thus we have, by the discussion in the previous chapter,
\[ f(E[g_1[\Phi]], \ldots, E[g_n[\Phi]]) = 1 - \prod_{k=0}^{n} \Pr[A_{n-k} \land \ldots \land \overline{A}_{n-k+1}] = \Pr[\Phi \in \text{HORN-SAT}]. \]

The above correction seems to be specific to the random model for Horn satisfiability, which allows clauses of varying lengths.

To sum up: the mean-field approximation is true, modulo a correction that takes into account some particular features of the random model for Horn satisfiability.

15. Discussion. We have characterized the asymptotical satisfiability probability of a random \( k \)-Horn formula, and showed that it exhibits very similar behavior to the one uncovered experimentally in [24].

We have also displayed an “easy-hard-easy” pattern similar to the ones observed experimentally in the AI literature. In our case the pattern is fully explained by elementary properties of the queuing chain.

As for an explanation of the “critical behavior”, consider an intermediate stage \( i \) of \( \text{PUR} \) and let \( C_j \) be the set of clauses of \( \Phi_{i,j}^P \). It is clear that whether \( \text{PUR} \) accepts is dependent only on the number of clauses in \( C_1 \). The restriction on the clause length acts like a “dampening” perturbation (in that it eliminates the “clause flow into \( C_k \)”). The proof of Theorem 6.2 states that when \( k(n) \to \infty \), with high probability \( \text{PUR} \) accepts (if \( \Phi \) is satisfiable) “before the perturbation reaches \( C_1 \)”, therefore the satisfiability probability is the one from the uniform case. On the other hand, for any constant \( \ell \), with probability greater than 0 \( \text{PUR} \) does not halt during the first \( k \) iterations (for the exact value see [17]), and the dampening has a significant influence. Thus the explanation for the occurrence (and specific form of) critical behavior is a threshold property for the number of iterations of \( \text{PUR} \) on random satisfiable Horn formulas “in the critical region”.

A related, and somewhat controversial, open issue is whether random Horn satisfiability properly displays critical behavior. Problems with a sharp threshold display “critical” (i.e. singular) behavior at least in one parameter, the satisfaction probability, which conceivably allows the definition of critical exponents. This is not so for random \( k \)-Horn satisfiability, that has a coarse threshold, and no criticality for \( k > 2 \), hence the question seems not to be meaningful. Note, however, that the order parameter involved in the recent study of the phase transition in 2-SAT [6] is not satisfaction probability, but the (expected size) of the so-called backbone (or its more tractable version spine) of a random formula. The “window” that we use to peek at the threshold behavior of random Horn satisfiability does not seem to be “naturally required” by any physical considerations, and it is possible in principle that the random Horn formulas display critical behavior if we take the spine as the order parameter.

16. Acknowledgments. This paper is part of the author’s Ph.D. thesis at the University of Rochester. Support for this work has come from the NSF CAREER Award CCR-9701911 and the NSF Grant 9725021.

REFERENCES

[1] D. Achlioptas, C. Gomes, H. Kautz, and B. Selman, Generating Satisfiable Problem Instances. In Proceedings of AAAI 2000, (to appear).
[2] N. Alon, P. Erdős, and J. Spencer. The probabilistic method. John Wiley and Sons, second edition, 1992.
[3] A. Barbour, L. Holst, and S. Janson. Poisson Approximation. Clarendon Press Oxford, 1992.
[4] J. Baxter. Exactly solvable models in Statistical Mechanics. J. Wiley and Sons, 1984.
[5] B. Bollobás. Random Graphs. Academic Press, 1985.
[6] B. Bollobás, C. Borgs, J.T. Chayes, J. H. Kim, and D. B. Wilson. The scaling window of the 2-SAT transition. Technical report, Los Alamos e-print server, http://xxx.lanl.gov/ps/math.CO/9909031, 1999.

[7] B. Bollobás and A. Thomason. Threshold functions. *Combinatorica*, 7(1):35–38, 1986.

[8] P. Cheeseman, B. Kanefsky, and W. Taylor. Where the really hard problems are. In *Proceedings of the 11th IJCAI*, pages 331–337, 1991.

[9] E. Friedgut. Necessary and sufficient conditions for sharp thresholds of graph properties, and the k-SAT problem. with an appendix by J. Bourgain. *Journal of the A.M.S.*, 12:1017–1054, 1999.

[10] A. Frieze and S. Suen. Analysis of two simple heuristics for random instances of k-SAT. *Journal of Algorithms*, 20:312–355, 1996.

[11] I. Gent, E. MacIntyre, P. Prosser, and T. Walsh. The scaling of search cost. In *Proceedings of AAAI-97*, pages 315–320, 1997.

[12] G. Grimmett. *Percolation*. Springer Verlag, 1988.

[13] Hara and G. Slade. Mean-field critical behaviour for percolation in high dimensions. *Communications in Mathematical Physics*, 128:333–391, 1990.

[14] B. Hayes. Can’t get no satisfaction. *American Scientist*, 85(2):108–112, March–April 1997.

[15] P. Hoel, S. Port, and C. Stone. *Introduction to stochastic processes*. Waveland Press Inc., 1987.

[16] T. Hogg and D. Mammen. A new look at the easy-hard-easy pattern of combinatorial search difficulty. *Journal of Artificial Intelligence Research*, 7:44–66, 1997.

[17] G. Istrate. The phase transition in random Horn satisfiability and its algorithmic implications. Submitted to Random Structures and Algorithms (journal version of paper that appeared in AIM’98 and SODA’99), available as Technical Report cs.DS/9912001, A.C.M. Computing Research Repository (CoRR), http://xxx.lanl.gov/, 1999.

[18] H. Kautz and B. Selman. Knowledge compilation and theory approximation. *Journal of the ACM*, 43(2):193–224, 1996.

[19] S. Kirkpatrick, C.D. Gelatt, and M. Vecchi. Optimization by simulated annealing. *Science*, 220(4598):671–680, 1983.

[20] S. Kirkpatrick and B. Selman. Critical behavior in the satisfiability of random boolean expressions. *Science*, 264:1297–1301, 1994.

[21] S. Kirkpatrick and B. Selman. Critical behavior in the computational cost of satisfiability testing. *Artificial Intelligence*, 81, 1996.

[22] J. Komlós and E. Szemerédi. Limit distribution for the existence of Hamiltonian cycles in a random graph. *Discrete Mathematics*, 43(1):55–63, 1983.

[23] T. Lindvall. *Lectures on the coupling method*. John Wiley, 1992.

[24] M. Mézard and G. Parisi. Replicas and optimization. *J. Phys. France*, 46:L771–L778, September 1985.

[25] M. Mézard, G. Parisi, and M. Virasoro. *Spin glass theory and beyond*. World Scientific, 1987.

[26] R. Monasson and R. Zecchina. Statistical mechanics of the random k-SAT model. *Physical Review E*, 56:1357, 1997.

[27] R. Monasson, R. Zecchina, S. Kirkpatrick, B. Selman, and L. Troyansky. 2 + p-SAT: Relation of typical-case complexity to the nature of the phase transition. *Random Structures and Algorithms*, 15(3–4):414–435, 1999.

[28] R. Monasson, R. Zecchina, S. Kirkpatrick, B. Selman, and L. Troyansky. Determining computational complexity from characteristic phase transitions. *Nature*, 400(8):133–137, 1999.

[29] C.M. Newman and D.L. Stein. Non-mean-field behavior of realistic spin glasses. *Physical Review Letters*, 76:515 – 518, 1996.

[30] C.M. Newman and D.L. Stein. Response to Parisi’s comment on “Non-mean-field behavior of realistic spin glasses”. Technical Report adapt-org/9603001, Los Alamos e-print server, http://xxx.lanl.gov/ps/adapt-org/9603001, 1996.

[31] G. Parisi. Recent results support the predictions of spontaneously broken replica symmetry for realistic spin glasses. Technical Report cond-mat/9603101, Los Alamos e-print server, http://xxx.lanl.gov/ps/cond-mat/9603101, 1996.

[32] S. Sheu. The Poisson approximation to the binomial distribution. *The American Statistician*, 38(3):206–207, 1984.

[33] M. Talagrand. Verres de spin et optimisation combinatoire. Seminaire Bourbaki. To appear in Asterisque., 1999.

[34] D.B.. Wilson. The empirical values of the critical k-SAT exponents are wrong. arXiv preprint math.PR/0005136 available from http://xxx.lanl.gov.