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Percolation of unsatisfiability in finite dimensions

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The satisfiability and optimization of finite-dimensional Boolean formulas are studied using percolation theory, rare region arguments, and boundary effects. In contrast with mean-field results, there is no satisfiability transition, though there is a logical connectivity transition. In part of the disconnected phase, rare regions lead to a divergent running time for optimization algorithms. The thermodynamic ground state for the NP-hard two-dimensional maximum-satisfiability problem is typically unique. These results have implications for the computational study of disordered materials.

Complex problems with many degrees of freedom are of interest to both physicists and theoretical computer scientists. The overlap is especially strong between the physics of disordered materials and optimization problems in the typical case. For example, there is a close correspondence between the ground states of Ising spin glasses, with up and down spins, and optimal assignments of Boolean variables, which can be true or false, in a logical formula. This correspondence is more than superficial as both systems exhibit phase transitions in the structure of minimal configurations and in the dynamics of the physical systems or optimization algorithms [1]. Such connections lead to advances in the two fields. Combinatorial optimization algorithms from computer science are often employed to simulate disordered condensed matter systems [2]. Approaches from statistical physics, including techniques such as replica theory and concepts such as the thermodynamic limit and scaling, have proven useful in studying the running time algorithms and the structure of solution space [3].

Motivated by work on mean field Boolean formulas and progress in understanding models of finite-dimensional disordered materials, we investigate ensembles of Boolean formulas whose graphs are two-dimensional. These formulas are composed by conjunctively joining logical clauses, with each clause formed using nearest neighbor variables. The optimization problem is to assign truth values so as to satisfy the maximum number of clauses in the formula. This is closely analogous to minimizing the number of broken bonds in an Ising spin glass [4]. Using ideas from statistical physics, including percolation and thermodynamic ground states, we find a transition in the structure of logically connected components and investigate the uniqueness of optimal assignments.

Decomposing the problem into clusters of strongly connected components that contain contradictory cycles greatly reduces the running time of an exact optimization algorithm. These contradictory strongly-connected components (CSC's) need not percolate even though the clauses form percolative structures. In addition, the rapid convergence to a unique ground state as the size of the problem increases suggests that the problem is easy in the typical case, though it is classified as difficult

in the worst case sense. Two central categories in this classification from computational complexity theory are P and NP decision (yes/no) problems [5]. Problems in P can be *decided* in time polynomial in the size of the problem description, while a proof of the answer for NP problems can be *checked* in polynomial time. NP-hard problems, a solution to which could be used to quickly solve any problem in NP, are believed to be solvable only in exponential time for the worst case realizations. It may well be that many NP-hard problems derived from physical systems, such as finding the ground state configuration for the 2D spin-glass in a magnetic field [6], are typically solvable in polynomial time. Our results support this possibility. NP-hard problems with algorithms that typically take polynomial time on some problem sets are known [5], but have not been extensively and directly studied for physical problems in finite dimensions.

We consider finite-dimensional Boolean formulas Z of the form

$$Z = \bigwedge_{\ell=1}^M (\bigvee_{i=1}^K y_i^\ell) \quad (1)$$

where \vee is the logical OR operation, \wedge is the logical AND operation, and $\{y_i^\ell\}$ are *literals* chosen from a set $Y = \{x_1, \dots, x_N, \bar{x}_1, \dots, \bar{x}_N\}$ of N Boolean *variables* and their negations. The variables are identified with the vertices of a two-dimensional lattice. We specialize to clauses with $K = 1$ and $K = 2$. We form 2-clauses by choosing two neighboring variables and negating each variable with probability 1/2. The 1-clauses are single literals, with probability 1/2 of negation. A sample formula is depicted in Fig. 1(a). The ensemble is defined by parameters α and γ , respectively the ratios of the number of 2-clauses to N and 1-clauses to N . The 2-clauses do not overlap and no two 1-clauses contain the same variable. Given a truth assignment $x_i \rightarrow \{T, F\}$ for all Boolean variables, a clause is satisfied if one of the literals in the clause is T . If all clauses are satisfied, the formula Z is satisfied. Determining the existence of a satisfying truth assignment is the problem of satisfiability (SAT).

The optimization of the number of satisfied clauses in Z can be mapped to determining the ground state of a spin glass in a heterogeneous field. This mapping translates Boolean assignments $x_i = \{F, T\}$ to spin variables

$S_i = \{-1, +1\}$. A bond energy E_ℓ can be assigned to a clause $(y_0^\ell \vee y_1^\ell)$ connecting variables x_i and x_j via [3]

$$E_\ell = \frac{J}{4}[1 - \Delta(y_0^\ell)S_i - \Delta(y_1^\ell)S_j + \Delta(y_0^\ell)\Delta(y_1^\ell)S_iS_j], \quad (2)$$

where $\Delta(y_0^\ell) = 1$ if $y_0^\ell = x_i$ and $\Delta(y_0^\ell) = -1$ if $y_0^\ell = \bar{x}_i$ and similarly for j (nearest neighbor to i) replacing 0 with 1. The total spin glass energy E is given by $E = \sum_{\ell=1}^M E_\ell$. Any clause that is not satisfied costs an energy J ; the existence of an $E = 0$ ground state is equivalent to satisfiability of the Boolean formula.

Resolution [5] is a method that can be used to quickly decide SAT for $K \leq 2$. This procedure is equivalent to mapping each 2-clause to a pair of logical implications and searching for “contradictory cycles” (CCs). For example, the clause $x_1 \vee x_2$ is equivalent to $\bar{x}_1 \rightarrow x_2$ and $\bar{x}_2 \rightarrow x_1$. Clauses with $K = 1$ are replaced by a single implication, e.g., \bar{x}_1 becomes $x_1 \rightarrow \bar{x}_1$. The Boolean formula can be represented by an implication digraph (i.e., directed graph) $G = (Y, E)$ with $2N$ vertices and $(2\alpha + \gamma)N$ edges E . For a sample mapping, see Fig. 1(b). The formula Z can not be satisfied if there is a CC, which is a path p in G that connects a variable to its negation and vice versa, i.e., $p = (x_i \rightarrow x_j \dots \rightarrow \bar{x}_i \rightarrow \dots \rightarrow x_i)$. For the formulas we consider, the existence of contradictory cycles can be decided in time linear in N [7].

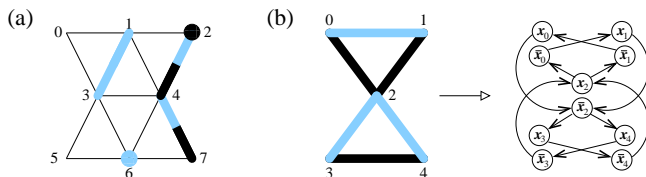


FIG. 1: (a) Example finite-dimensional Boolean formula. Each 2-clause in the formula is an edge, represented by two segments. Circles represent 1-clauses. Black segments or circles indicate negated variables, while the lighter shaded segments or circles represent variables that are not negated. The formula depicted is $(x_1 \vee x_3) \wedge (x_2 \vee \bar{x}_4) \wedge (x_4 \vee \bar{x}_7) \wedge (\bar{x}_2) \wedge (x_6)$. (b) A smallest unsatisfiable subgraph for the triangular lattice (left) and its digraph (right). The subgraph’s formula is $(x_0 \vee x_1) \wedge (\bar{x}_0 \vee \bar{x}_2) \wedge (\bar{x}_1 \vee \bar{x}_2) \wedge (x_2 \vee x_3) \wedge (x_2 \vee x_4) \wedge (\bar{x}_3 \vee \bar{x}_4)$. A contradictory cycle (CC), in this digraph is $x_2 \rightarrow \bar{x}_0 \rightarrow x_1 \rightarrow \bar{x}_2 \rightarrow x_3 \rightarrow \bar{x}_4 \rightarrow x_2$.

We find that there are CCs for any $\alpha > 0$ (taking $\gamma = 0$), as $N \rightarrow \infty$, in these finite-dimensional formulas. Defining $\alpha_{1/2}(N)$ as the value of α for which 1/2 of the finite-dimensional N -variable formulas are satisfiable, $\alpha_{1/2}(N) \rightarrow 0$ as $N \rightarrow \infty$ (see Fig. 2.) This crossover is coarse, in that the width of the crossover from low to high probability of satisfiability is proportional to $\alpha_{1/2}(N)$, for large N . This to be contrasted with random mean-field $K = 2$ formulas, where for $N \rightarrow \infty$, there is a sharp SAT to UNSAT phase transition (the probability that a formula is satisfiable is 1 for $\alpha < \alpha_c = 1$ and 0 for larger α .)

These differences result from small CCs, which at small α are exponentially rare in the mean field case but appear with Poissonian statistics in the finite-dimensional case, where loops are more important.

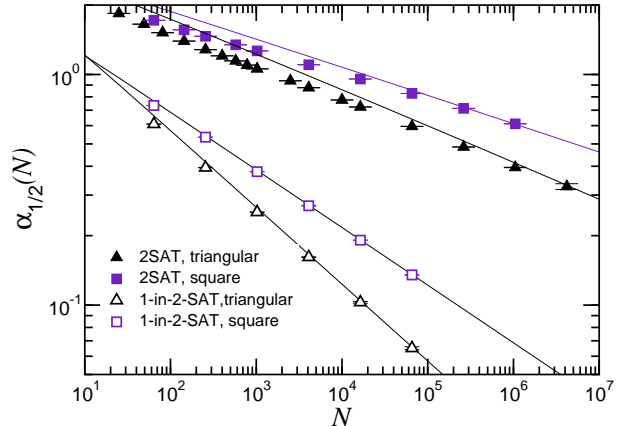


FIG. 2: (a) Plot of $\alpha_{1/2}(N)$, the clause density at which 1/2 of the graphs are satisfiable, as a function of lattice size N . Symbols indicate numerical results for 2SAT and 1-in-2-SAT (Ising spin glass) on triangular and square lattices. Curves are analytic approximations found in a small subgraph expansion.

The location of the SAT/UNSAT crossover can be computed by an expansion in α . Some subgraphs are “forcing”, i.e., in all satisfying assignments one of the variables has a fixed truth value. The smallest unsatisfiable graph is found by joining two contradictory forcing subgraphs. An example of this graph type is depicted in Fig. 1(b). On the triangular lattice, these subgraphs have density $\rho_\Delta(\alpha) = \frac{\alpha^6}{273^4} + \mathcal{O}(\alpha^7)$. The density of the simplest unsatisfiable graphs on the square lattice is $\rho_\square(\alpha) = \frac{\alpha^8}{216} + \mathcal{O}(\alpha^9)$. In general, if the smallest unsatisfiable subgraph has r bonds and density $c_r \alpha^r$, the probability of satisfiability is $P_{\text{SAT}}(N) = (1 - c_r \alpha^r)^N$, to lowest order in α , giving $\alpha_{1/2}(N) \approx (c_r^{-1/r} \ln 2) N^{-1/r}$. We plot numerical results and analytic expansions for $\alpha_{1/2}(N)$ in Fig. 2, which includes the next order analytic corrections in α (7-edged subgraphs with density $\frac{5^2}{273^7} \alpha^7 + \mathcal{O}(\alpha^8)$ on the triangular lattice and 9-edged subgraphs with density $\frac{\alpha^9}{216} + \mathcal{O}(\alpha^{10})$ on the square lattice).

We also plot analytic estimates and numerical results for $\alpha_{1/2}(N)$ for the 1-in-2-SAT problem in Fig. 2. While a clause in 2SAT (i.e., $K = 2$) is satisfied if either literal is true, a clause is satisfied in 1-in-2-SAT when exactly one literal in a clause is true. The 1-in-2-SAT problem maps both to an Ising spin glass in the absence of a magnetic field and to the two-color problem [8]. The smallest unsatisfiable graphs are given by frustrated cycles, giving $\alpha_{1/2}(N) \approx 3(N/\ln 2)^{-1/3}$ and $\alpha_{1/2}(N) \approx 2^{5/4}(N/\ln 2)^{-1/4}$ for the triangular and square lattices, respectively.

Given the lack of a sharp SAT/UNSAT transition, due

to the existence of *small* unsatisfiable graphs, we have investigated the percolation of *large* unsatisfiable graphs as a phase transition. We study these graphs within the context of MAXSAT, which is the problem of minimizing the number of unsatisfied clauses. In two dimensions, the determination of the ground state for the Ising spin glass (or MAX-1-in-2-SAT) is in P [6], while determining the ground state for MAXSAT with $K = 2$ is NP-hard, even for planar graphs. We studied the CSCs, sets of literals for which any two literals are connected by a directed path in the implication digraph and which contain a CC. We find that the probability of having a spanning CSC has a transition that becomes sharper with increasing N , with a critical value for α of $\alpha_S = 1.8245(5)$ on the triangular lattice. The cluster size distribution $n(s)$ at criticality behaves as $n(s) \sim s^{-\tau}$, with $\tau = 2.02(5)$. The scaling of the probability for a spanning CSC near α_S gives a correlation length exponent of $\nu = 1.32(3)$. These values are consistent with the 2D values for standard percolation, where $\tau = 187/91$ and $\nu = 4/3$ [9].

Percolation of paths in the implication digraph can be related to connectivity percolation [10]. This is done by projecting part of the implication digraph on $2N$ literals onto an undirected graph of N variables. This “trimmed” projection has the same statistics as standard connectivity percolation with edge probability $\tilde{p} = 2p - p^2$, where for our finite-dimensional case, $p = \alpha/2z$, with $z = 4$ ($z = 6$) for square (triangular) lattices, if overlapping clauses are allowed. (On the triangular lattice with overlapping clauses, we find $\alpha_S = 1.887(2)$.) In mean field, the percolation of paths containing a contradiction coincides with the SAT/UNSAT transition. This is not the case in finite dimensions. But given this type of connection and studies of percolation of directed edges in finite dimensions [11], it is not surprising that CSC percolation appears to be in the same universality class as standard connectivity percolation.

The decomposition of the graphs into CSCs speeds up exact search algorithms for MAXSAT. Here, we apply this decomposition to estimate running times of such an algorithm. We used a MAXSAT code [12] that first finds a heuristic bound to the solution and then applies an exact Davis-Putnam-Loveland-Logemann (DPLL) search. The running time measure t is the number of “backtracks” that are executed while partially exploring the tree of all possible assignments. Each CSC cluster can be loaded into the algorithm individually [13]. The sum of the unsatisfied clauses from each cluster gives the minimal number of unsatisfied clauses for the entire formula. When $\alpha < \alpha_S$, the distribution of sizes of the CSCs, is exponentially decaying in the cluster size, $n(s) \sim e^{-s/s_\xi(\alpha)}$, with $s_\xi \propto \xi^d \propto (\alpha_S - \alpha)^{-d\nu}$. If we plot the median number of backtracks for each cluster, we find that the median running time of the DPLL-type algorithm scales exponentially with the cluster size, $t^*(s) \sim e^{s/s_\tau(\alpha)}$. When $s_\xi(\alpha) < s_\tau(\alpha)$, the median running time for a sample,

$T^*(L)$, is bounded by a multiple of the system volume, $T^*(L) \sim L^2$. However, when $s_\xi > s_\tau$, $T^*(L)$ diverges more rapidly, with an estimate for the largest cluster size in a finite sample giving $T^*(L) \sim L^{2s_\tau/s_\xi}$. The mean running time, $\bar{T}(L)$, diverges exponentially with L . The transition between the linear and superlinear median time behaviors defines $\alpha_G < \alpha_S$ via $s_\xi(\alpha_G) = s_\tau(\alpha_G)$. Fig. 3 shows convolutions of the cluster size distribution $n(s)$ and the median time $t^*(s, \alpha)$ as a function of size. The change from negative to positive slope on the semi-log plot gives $\alpha_G \approx 1.3$ for the DPLL code we use. This slowing down of the algorithmic dynamics is similar to that for the physical dynamics of random magnets [14] and is reminiscent of the change from the easy-SAT to hard-SAT phases in random graphs [1].

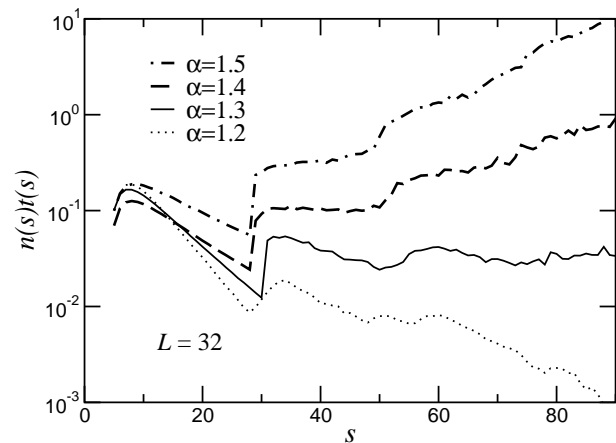


FIG. 3: Convolution of the median number of backtracks $t^*(s)$ with the CSC cluster size distribution $n(s)$, where s is the cluster mass. Note that $\alpha < \alpha_S$ for these curves.

Despite the divergence of the running times for the exhaustive DPLL-type algorithms, we might expect that the ground states could be found in time proportional to the system volume in the typical case, even above the CSC percolation transition. Assuming that the droplet picture describes these finite-dimensional spin glasses, the presence of the magnetic field destroys the spin glass phase [15] and the correlations are finite-ranged (though in 2SAT there are some correlations in the external fields.) So while the CSCs percolate, the effects of frustration remain localized beyond some length scale. This picture also implies one unique thermodynamic state. If this is the case there may be a way to develop a new algorithm to deal with the local frustrated bonds, either by solving subsystems and joining the solutions together to form the whole system or by a more clever heuristic algorithm. We leave this as a conjecture and simply test for uniqueness.

To test whether the ground state is unique, we study the effect of boundary conditions, similar to studies of the Ising spin glass [16]. By comparing ground states for a

system of linear size L and an expanded system of linear size L' (each with free boundaries), one can determine if the ground state is unique or not from the sensitivity to boundary conditions. If the solutions in the common subsystem of linear size w become fixed as L and L' diverge, a unique ground state exists in the thermodynamic limit. Note that the ground state must be unique for $\alpha < \alpha_S$, as the logical structure of the graph does not percolate.

Since the $\pm J$ spin glass with magnetic field (equivalent to optimal assignments for MAX2SAT) has many degenerate ground states, we study the weighted MAX2SAT (WMAXSAT) question, where the degeneracy is broken, to be able directly to compare ground state solutions. Each clause has an associated weight, chosen uniformly in the interval $[0, 1)$, and the optimization problem is now to minimize the sum of the weights of the unsatisfied clauses. We also introduce 1-clauses, with the same weight distribution. The addition of 1-clauses lowers α_S , allowing us to study a larger range system of system sizes, as the graphs are sparser.

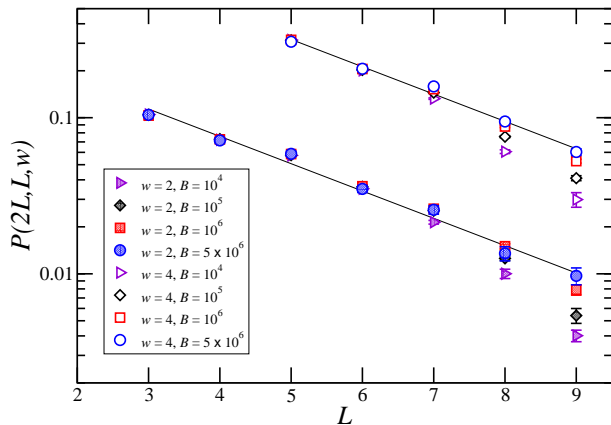


FIG. 4: Log-linear plot of $P(2L, L, w)$ for $\alpha = 1.7$ and $\gamma = 0.2$ for weighted MAX2SAT. The bound on backtracks is B . The lines are exponential fits for the $w = 2, 4, B = 5 \times 10^6$ data.

We estimate the quantity $P(2L, L, w)$, the probability that there is a change in the central area of area w^2 when the system size expands from L to $2L$ [16], by sampling from the WMAXSAT ensemble. To be able to complete the simulations, we impose an upper limit B on the number of backtracks in the DPLL and report P for a range of B . The points in Fig. 4, with $w = 2$, are well fit by an exponential in L , in the limit of large B . (A power law fit gives an exponent less than -2 , which is inconsistent with a fractal domain wall picture for a model with two states [16].) The $w = 4$ data is also well described by an exponential with the same slope. For $\alpha = 1.7$ and $\gamma = 0.2$, we estimate a correlation length of $\xi = 2.5 \pm 0.3$. The exponential approach to a unique state holds for all α and γ that we explored.

Working within the concepts and the algorithms for

spin glasses and other disordered materials, we have studied the problem of optimal satisfaction of Boolean formulas. There is no thermodynamic SAT to UNSAT transition, due to the finite density of small unsatisfiable formulas. There is a percolation transition, however, in the logical structure of the formulas as the clause density is increased, that is apparently in the class of standard connectivity percolation. Below this transition, we use rare region arguments to predict a transition in the mean running time of an optimization algorithm. We find that the ground state is unique even in the high clause density regime. This uniqueness suggests that the MAX2SAT problem can be solved “locally” by studying subsamples larger than the correlation length and patching subsolutions together (though for large correlation lengths, rare regions might again dominate the running time.) This general approach in turn has potential applications to algorithms for studying spin glasses and other random magnets. This project was supported in part by the National Science Foundation through grant DMR-0109164.

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