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Weixiong Zhang

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1 Introduction and Overview

Understanding phase transition phenomena in complex systems and combinatorial problems [3, 9–11, 13, 14, 20, 21] has been an active research focus for more than a decade. It is now well known that Boolean satisfaction problems typically exhibit easy-hard-easy phase transitions [3, 14]. Specifically, the computational complexity of 3-SAT, a Boolean satisfaction problem in a conjunctive normal form with three literals (variable or its negation) per clause, experiences dramatic transitions from easy to difficult and then from difficult back to easy when the ratio of the number of clauses to the number of variables increases. Note that 3-SAT is a decision problem, which gives a solution when the problem is satisfiable or an answer NO when it is unsatisfiable.

On the other hand, it has also been shown that the expected complexity of finding optimal solutions of tree search problems, which include many of those combinatorial optimization problems that are solved by branch-and-bound, goes through easy to difficult transitions when the underlying heuristic function degenerate [11, 13, 20, 21].

In short, the phase transitions of NP-complete decision problems have easy-hard-easy patterns and the phase transitions of NP-hard optimization problems follow easy-hard patterns. These phase transition results exhibit a discrepancy between the phase transitions of decision and optimization problems.

An example of such a discrepancy is explicitly shown in two independent experimental study of phase transitions of the Traveling Salesman Problem (TSP) [8, 22]. It was shown that there exists a rapid transition between soluble and insoluble instances of the decision problem of two-dimensional Euclidean TSP, and hard instances are associated with this transition, showing an easy-hard-easy pattern [8]. On the other hand, it was shown that the complexity of finding optimal solutions to the TSP displays an easy-hard pattern [22].

Phase transitions of different problems have different control or order parameters that may be adjusted to alter the phases of the problems. For instance, an order parameter for 3-SAT is the ratio of the number of clauses to the number of variables [3, 14] and the number of distinct values of intercity distances is an order parameter for the TSP [22].

A more profound concept related to phase transitions is that of the backbone, which has been suggested as a more pertinent order parameter to characterize a complex problem. A *backbone* of a combinatorial problem is a set of variables each of which has the same value among all solutions [15]. In other words, backbone variables are extremely constrained. A violation to a backbone variable rules out all optimal solutions.

This research was first motivated by the fact that there are numerous real-world constraint problems for which not all constraints can be satisfied. Such problems can be found in application areas such as scheduling, multi-agent co-operation and coordination, and pattern recognition [2, 4, 6]. Given such an over-constrained problem, the task of finding an solution to minimize the total number of violated constraints is an optimization problem, which we call *constraint minimization problem* (CMP).

We are also motivated to understand the relationship between the phase transitions of decision problems and that of their optimization counterparts. In this study, we will focus our investigation on 3-SAT, which is a decision problem, and MAX 3-SAT, which is an optimization problem that requires the optimal solutions minimizing the total number of unsatisfied constraints.

Furthermore, We are motivated to investigate the backbones of optimization problems, particularly the backbone of MAX 3-SAT. Our goal is to understand the characteristics of all optimal solutions and the behavior of finding them.

The paper is organized as follows. After a brief review of 3-SAT and MAX 3-SAT, we examine the phase transitions of 3-SAT and MAX 3-SAT by showing their different phase transition patterns (Section 2.2). We then generalize the notion of satisfiability to different decision problems with various bounds on decision quality (Section 2.3). We then study the backbone of MAX 3-SAT (Section 3). We discuss related work in Section 4 and conclude in Section 5.

2 Decision vs. Optimization Phase Transitions

In this section, we experimentally analyze the relationship between the phase transitions of decision problems and that of optimization problems. Our discussion will focus on 3-SAT and MAX 3-SAT.

In our experiments on 3-SAT and MAX 3-SAT, we used 25 variables and varied the number of clauses to generate random problem instances. In generating a clause, a randomly chosen variable has a 50 percent chance to be negated. No duplicate clause is allowed in a problem instance. We varied the clause/variable ratio from 1 to 20, with an increment of 0.2. For each clause/variable ratio, we generated 1,000 problem instances. We collected the median value or computed an averaged value of the results on these instances as needed.

In this study, we used the well-known Davis-Putman method, a backtracking method with unit resolution [5]. This algorithm is a special case of depth-first branch-and-bound where one variable is instantiated at each step.

2.1 3-SAT and MAX 3-SAT problems

A *Boolean satisfiability*, or *SAT* for short, is a constraint satisfaction problem (CSP) that involves a Boolean formula consisting of a set of Boolean variables and a conjunction of a set of disjunctive clauses of literals, which are variables and their negations. A clause is satisfied if a literal within it takes a true value, and a Boolean formula is satisfied if all the clauses are satisfied. The conjunction defines constraints on the possible combinations of variable assignments. A *3-SAT* is a special Boolean satisfiability where each clause has three literals. 3-SAT is NP-complete [7], and it is unlike to have a polynormial algorithm for the problem. Many practical problems can be cast as SAT [6, 19].

Furthermore, there are also practical SAT problem in which no variable assignments can be found which does not violate a constraint [6]. In this case, it is required to find an assignment such that the total number of satisfied clauses is maximized. This is called *maximum 3-Sat*.

2.2 Discrepancy of phase transitions

As discussed in Section 1, there is a discrepancy between the phase transitions of decision problems and the phase transitions of their corresponding optimization versions. We investigate this discrepancy in detail.

We first consider 3-SAT. Figure 1 shows two types of phase transitions, a transition between satisfiability and unsatisfiability and easy-hard-easy transitions of computation cost. The order parameter that determines the phase transitions is the ratio of the number of clauses to the number of variables. The critical value of this order parameter for 3-SAT is around 4.13 [14]. A 3-SAT is almost always satisfiable when the clause/variable ratio is below this critical value and is almost always unsatisfiable when the ratio is beyond the critical value, making a sharp transition from satisfiability to unsatisfiability. Furthermore, the computational complexity required to decide the satisfiability is low when the probability of satisfiability is close to one or zero; while the complexity is the highest when this probability is 0.5, a value taken when the clause/variable ratio is around 4.13.

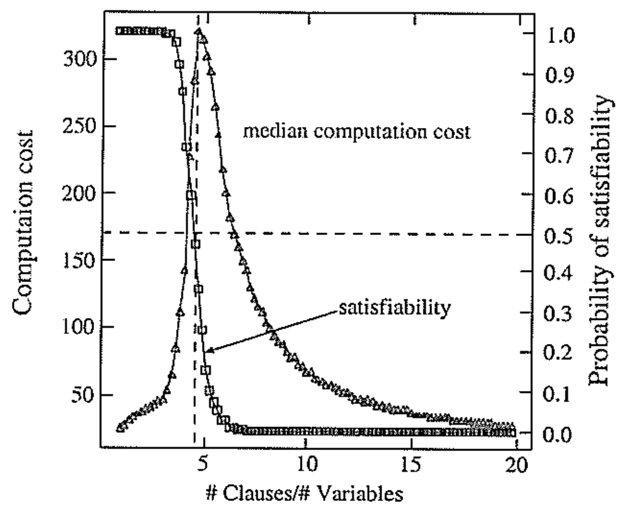

Fig. 1. Phase transitions of 3-SAT.

We now consider MAX 3-SAT. The only property we need to consider is its computational complexity, since an optimal solution is required throughout the whole spectrum of consideration so that there is no notion of satisfiability for the problem. Figure 2 shows the complexity of solving random MAX 3-SAT with 25 variables and various numbers of clauses. The problem instances used in Figure 2 are the same as that in Figure 1. To contrast the result with 3-SAT, we also include the complexity curve for 3-SAT. Figure 2 shows that starting at point A in the figure, MAX 3-SAT follows 3-SAT to enter computationally difficult region. However, MAX 3-SAT becomes more and more difficult when the clause/variable ratio increases even when 3-SAT enters its second easy region. In other words, the complexity of MAX 3-SAT follows an easy-hard pattern as the clause/variable ratio increases.

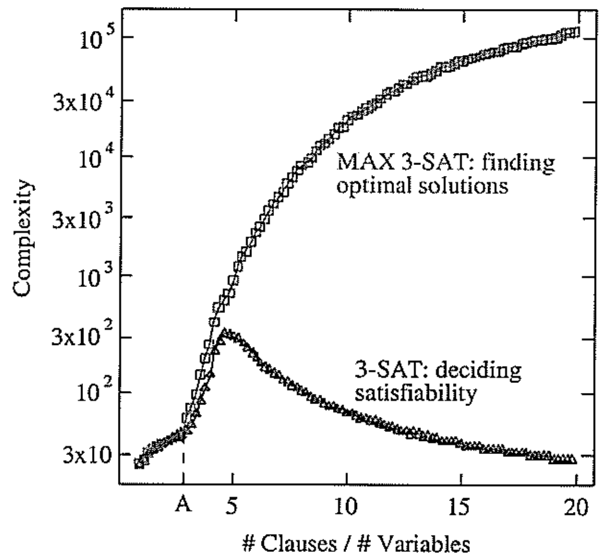

Fig. 2. Phase transitions of MAX 3-SAT.

The discrepancy between the different patterns of the complexity phase transitions of 3-SAT and MAX 3-SAT indicates that optimization is more difficult than decision. The optimal solution to a MAX 3-SAT can be obviously used to answer the question if the corresponding 3-SAT is satisfiable or not. Thus a MAX 3-SAT, a minimization problem, is at least as hard as its corresponding 3-SAT, a decision problem. This discrepancy also indicates that constraints play different roles in an optimization problem and in its decision counterpart. When a problem instance is satisfiable, deciding if it is satisfiable is to find a variable assignment satisfying all the constraints, which is also an optimal solution to the optimization version of the problem. When a constraint problem is overconstrained, a small subset of the problem is very likely to be overconstrained as well, so that the problem can be declared unsatisfiable when such an overconstrained subproblem is detected unsatisfiable. The more constrained the problem is, the more quickly the decision process can conclude that no solution exists. However, in an overconstrained case, finding an optimal solution to minimize the total number of violated constraints is typically hard since every possible variable assignment can be a candidate of a optimal solution.

2.3 Quality-bounded decision problems

The discrepancy between the two different phase transition patterns of 3-SAT and MAX 3-SAT has motivated us to investigate the relationship of the phase transitions of these two closely related problems.

In between a decision problem and its optimization counterpart there are many middle grounds that consist of decision problems with different decision objectives and quality. Such a decision problem may ask if there exists a variable assignment that violates no more than B constraints for an integer bound B. We call such a general decision problem *quality-bounded decision problem*, or *bounded decision problems* for short, and note it as 3-SAT(B). A 3-SAT(B) is satisfied if an assignment that violates no more than B constraints exists. It takes 3-SAT and MAX 3-SAT as special cases. When $B = 0$ it is 3-SAT; when B is the optimal solution cost, it is equivalent to MAX 3-SAT.

Are the phase transition properties of 3-SAT reserved under the general notion of satisfiability? Specifically, are there still a sharp transition from satisfiability to unsatisfiability and easy-hard-easy complexity transitions in 3-SAT(B) when the clause/variable ratio increases?

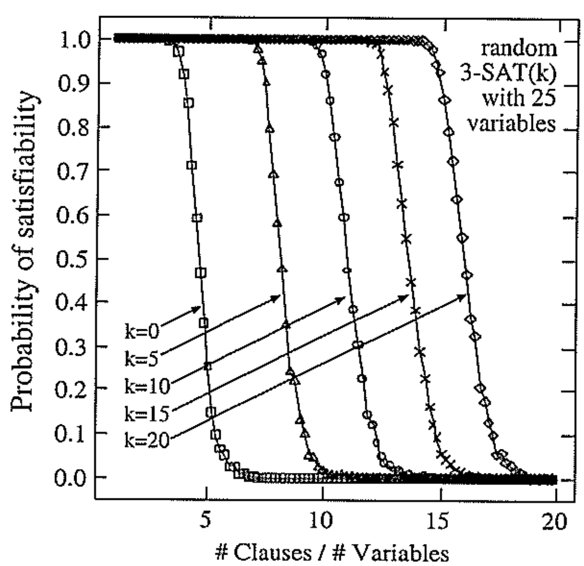

Fig. 3. Satisfiability phase transitions of 3-SAT(B).

Figures 3 and 4 show our experimental results that answer these questions. Figure 3 shows the probability of satisfiability of 3-SAT(0), 3-SAT(5), 3-SAT(10), 3-SAT(15), and 3-SAT(20). The figure shows that 3-SAT(B) still has a sharp transition from satisfiable to unsatisfiable as the clause/variable ratio increases.

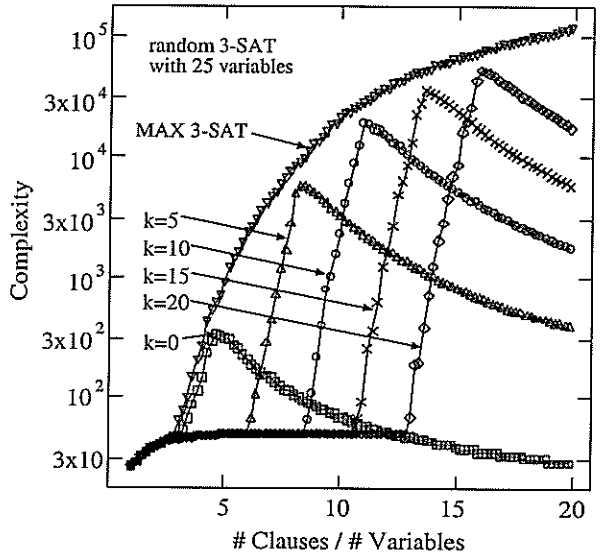

Fig. 4. Complexity phase transitions of 3-SAT(B).

The location of the transition for a given clause/variable ratio depend on B, however. The larger B is, the more problem instances are satisfiable. Similar to the unsettled issue of the exact location of the satisfiable to unsatisfiable transition of 3-SAT, it remains an interesting open problem to analytically determine the transition location of 3-SAT(B) with a non-zero integer bound B.

Figure 4 shows the computational complexity of Davis-Putman algorithm on 3-SAT(0), 3-SAT(5), 3-SAT(10), 3-SAT(15), 3-SAT(20), and MAX 3-SAT. Note that the vertical axis is in a logarithmic scale. As the curves in the figure show, although the complexity of 3-SAT(B) still follows an easy-hard-easy transition pattern, the second easy region where problem instances are overconstrained becomes no longer very easy comparing to the first easy region where the problems are underconstrained. The larger B is, the computationally more difficult the second easy region becomes.

In summary, a profound feature of phase transitions on computational complexity of 3-SAT(B) is that the transition from the first easy region to the difficult region is very sharp. In the first easy region, the computational complexity of 3-SAT(B) is relatively constant regardless the actual value of B. Whenever the complexity enters the difficult region, the complexity increases exponentially.

3 Phase Transitions of CMP Backbones

We now study the backbones of constraint minimization problems. In our experiments, we used the same set of randomly generated problem instances as for the experiments in the previous section. Specifically, we used 25 variables and varied the number of clauses by changing the clause/variable ratio from 1 to 20, with an increment of 0.2. For each clause/variable ratio, we generated 1,000 problem instances. We collected the median value or computed an averaged value of the results on these instances as needed.

Since backbone is defined over all solutions of a problem, we first examine the problem of finding all optimal solutions to MAX 3-SAT problems.

3.1 Finding all optimal solutions

It is known that there are a large number of satisfying solutions whenever 3-SAT is underconstrained, which are credited for the low computation cost in the underconstrained region. These satisfying solutions are also optimal solutions to MAX 3-SAT. When 3-SAT is overconstrained, however, a satisfiable solution is unlikely to exist. What is the total number of optimal solutions when MAX 3-SAT is overconstrained? How will the other two important characteristics, the cost of optimal solutions and the computational cost of finding all optimal solutions, behave?

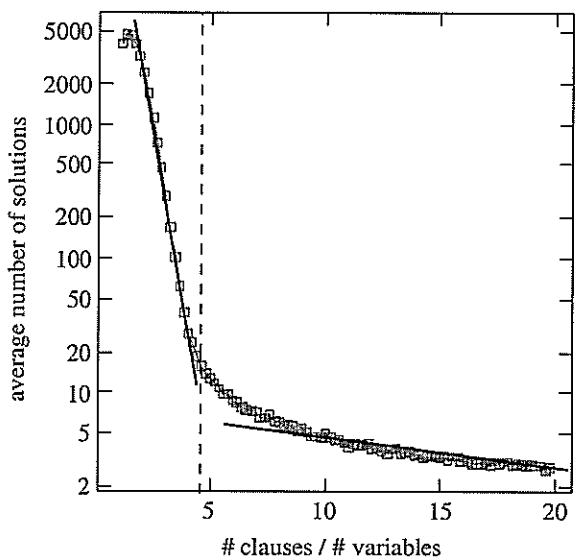

Fig. 5. Number of optimal solutions of MAX 3-SAT.

Figure 5 shows the average number of optimal solutions of MAX 3-SAT with 25 variables in terms of clause/variable ratio. The dotted line in the figure is where the 50 percent satisfiability of 3-SAT occurs. The vertical axis is in a logarithmic scale. As Figure 5 shows, the curve of the average number of optimal solutions can be divided into two segments. In the underconstrained region, the average number of solutions decreases *exponentially* as the clause/variable ratio increase. In the overconstrained region, the number of solutions is less than a dozen, and decreases approximately linearly with the clause/variable ratio.

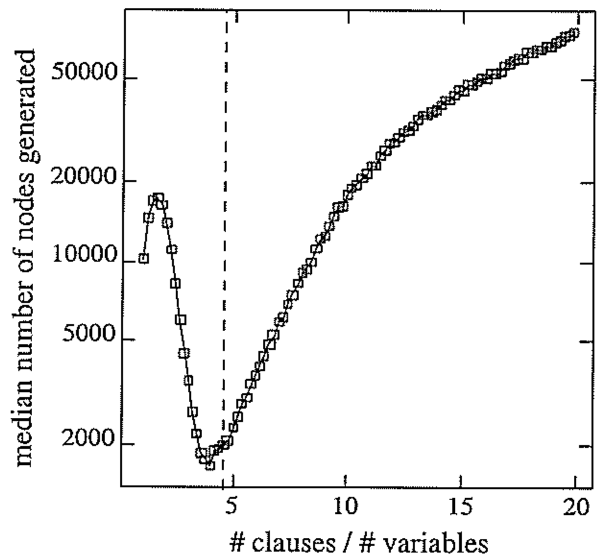

Fig. 6. Computational cost of MAX 3-SAT.

We now examine the computational cost of finding all optimal solutions of MAX 3-SAT. Figure 6 shows the experimental results. The median computational cost is shown in a logarithmic scale along the vertical axis. The computational curve is also separated by the 50 percent satisfiability point of 3-SAT, which is shown by the vertical dotted line in Figure 6. The major trend of the curve in the underconstrained region is an exponential drop. This differs significantly from the low, increasing computational cost for 3-SAT in this region as shown in Figure 1. The higher computational cost when the ratio is smaller is mostly due to enumerating the large number of optimal solutions (cf. Figure 5). The curve exhibits a small plateau near the 50 percent satisfiability point. When the clause/variable ratio passes through the 50 percent satisfiability separation point, the computational cost steadily increases exponentially.

If finding a single satisfiable solution to a 3-SAT at the 50 percent satisfiability point is considered difficult (cf. Figure 1), then finding all solutions of MAX 3-SAT is a much harder problem. Based on Figure 6, the cost for finding all solutions around the 50 percent satisfiability point is near the lowest.

Another characteristic factor associated with finding all solutions is the median cost of optimal solutions, which is shown in Figure 7. The cost curve also has two segments, separated again by the 50 percent satisfiability line, the dotted line in the figure. In the underconstrained region, the median number of violated clauses remains zero; while in the overconstrained region, the cost increases linearly with the clause/variable ratio.

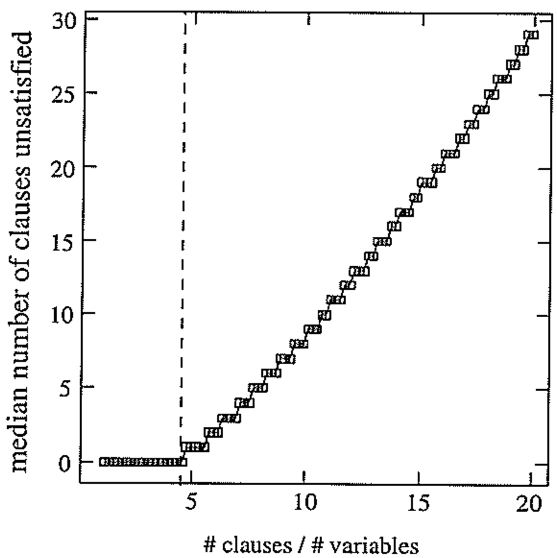

Fig. 7. Cost of optimal solutions of MAX 3-SAT.

In summary, the three main features associated with MAX 3-SAT, the number of optimal solutions, the computational cost for finding all solutions and the cost of optimal solutions, are segmented by the 50 percent satisfiability point of 3-SAT, and follow different patterns in the underconstrained and overconstrained regions.

3.2 Backbone phase transitions

A backbone of a 3-SAT is a fraction of variables of all the variables which have fixed values in all satisfying solutions [15]. In parallel, a backbone of a MAX 3-SAT is the fraction of variables of all the variables which have fixed values in all optimal solutions. In short, backbone variables are those critically constrained. A violation to any of these variables will rule out all optimal solutions.

The size of a backbone is measured by a real number ranging from 0 to 1. A backbone of 0 means that no variable is a backbone variable; while a backbone of size 1 means that all variables are backbone variables.

Our study of MAX 3-SAT backbones revealed two interesting and surprising results. First, there exist phase transitions of the backbones, shown in Figure 8,

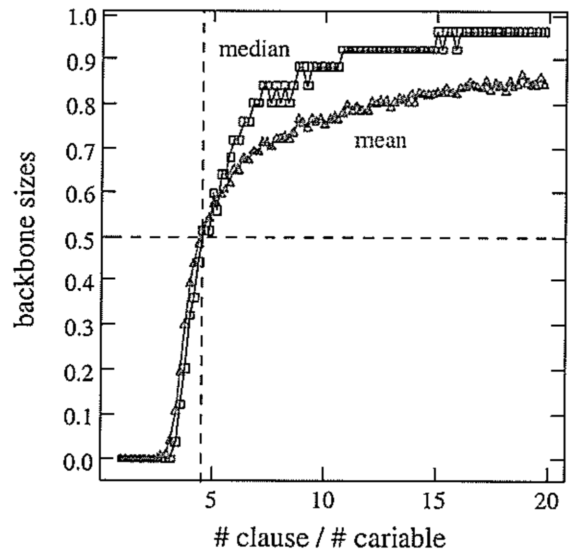

Fig. 8. Phase transitions of MAX 3-SAT backbones.

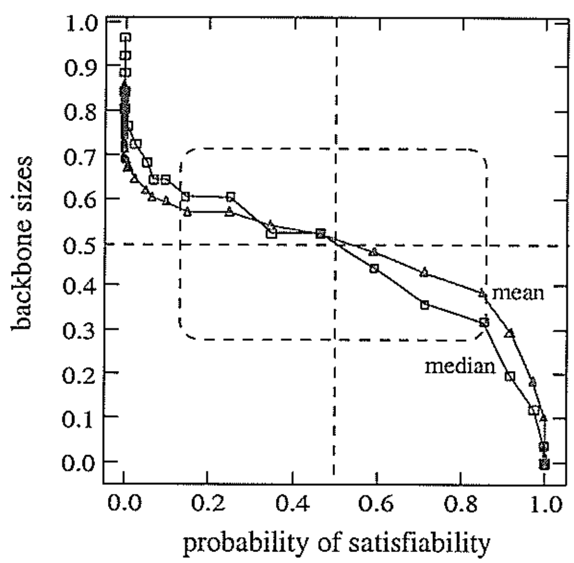

Fig. 9. Collocation of 0.5-0.5 transition points and near linear relation.

where the median size and average size of the backbones of 1,000 MAX 3-SAT problem instances are included. As the figure shows, backbones emerge abruptly as the clause/variable ratio increases. When the clause/variable ratio is less than 3.6, backbones almost do not exist. When the ratio is more than 3.6, backbones emerge quickly. Before the clause/variable ratio gets to 6, the median backbone size grows to more than 0.7, and reaches more than 0.9 when the ratio is 11.

The second surprising and more interesting result is that the backbone phase transitions of MAX 3-SAT are coincident with the satisfiability phase transitions of the corresponding 3-SAT. This is shown in Figure 9. The location where the backbone of MAX 3-SAT is 0.5 concurs approximately with the location where the corresponding 3-SAT has a probability 0.5 to be satisfiable. Within the vicinity near this 0.5-0.5 collocation (the dotted square within Figure 9), the backbone of MAX 3-SAT and the satisfiability of 3-SAT seem to be linearly correlated. An increase in backbone will cause the probability of satisfiability to drop proportionally, and vice versa.

There are only a few optimal solutions when the clause/variable ratio is very large, as shown by Figure 5. The backbone size is large when the clause/variable ratio is large, as shown in Figure 8. The combination of these two factors indicates that a handful of optimal solutions are clustered in a small neighborhood. Therefore, searching for any one of the clustered optimal solutions is difficult when backbone is large, since it is more likely to make a mistake of not setting a backbone variable to its correct value. On the other hand, when there exists no backbone variable, an arbitrary variable assignment may be an optimal solution. Therefore, finding such an optimal solution is easy.

4 Related Work

Huberman and Hogg discussed and argued that phase transitions are a universal feature of complex systems and problems [10]. Cheeseman et. al. [3] first experimentally demonstrated the existence of phase transitions in many combinatorial decision problems, including Boolean satisfiability, the Traveling Salesman Problem and graph coloring. The phase transitions of 3-SAT were extensively examined by Mitchell et. al. [14] and many other authors. This line of work concentrated mainly on decision problems. One of the main results is that the average computational complexity of decision problems follows an easy-hard-easy pattern.

The study of phase transitions of optimization problems probably started with Karp and Pearl's work of best-first search on a special random tree [11]. This random tree is an abstract model of many combinatorial search problems and state-space search algorithms, including best-first search and depth-first branch-and-bound. This work was extended to a more general tree by McDiarmid [13]. Zhang and Korf expanded the work to various linear space search algorithms, including depth-first branch-and-bound and iterative deepening [20, 21]. A main conclusion of this line of research is that the expected computational complexity of optimization problems exhibits an easy-hard pattern.

The discrepancy between the easy-hard-easy phase transitions of decision problems and the easy-hard transitions of optimization problems has inspired us to investigate the relationship of these two types of problems and their phase transitions closely in this research. One of the results of this research reconciles the relationship between the phase transitions of these two types of combinatorial problems.

Backbone seems to be an old concept, studied by Kirkpatrick and Toulouse on the Traveling Salesman Problem [12], and attracting much attention recently. Monasson et. al., investigated the backbones of 3-SAT and (2+p)-SAT and suggested backbone as an order parameter for the decision problems [15]. Achilioptas also considered the backbones of quasigroup complete problems [1]. Slaney and Walsh studied the backbones of many combinatorial optimization and approximation problems, such as graph coloring, the Traveling Salesman Problem, number partitioning and blocks world planning [18]. The relationship between backbone and local search on 3-SAT was studied by Parkes [16] and Singer et. al. [17].

Compared to the existing work on backbone, we made two main contributions in this research. The first is the result of the collocation of the 0.5 backbone of MAX 3-SAT (an optimization problem) and the 0.5 satisfiability of 3-SAT (a decision problem). The second is the result of the near linear correlation between these two phase transitions of two different but closely related problems.

5 Conclusions

We draw two conclusions from this research on constraint minimization problems. First, phase transitions are persistent in bounded 3-SAT (3-SAT(B)) in which up to B constraints may be violated. We showed that deciding if there exists a variable assignment with no more than B constraints unsatisfied exhibits similar phase transitions as that in 3-SAT, i.e., dramatic satisfiable to unsatisfiable transitions and easy-hard-easy computational complexity phase transitions. However, the difficulty of the second computationally easy phase in 3-SAT(B) increases with the quality bound B. Furthermore, the computational cost of MAX 3-SAT envelops the computational cost peaks of 3-SAT(B).

Second, the backbone of MAX 3-SAT also experiences a phase transition. A backbone is almost not existent in the underconstrained region, abruptly emerges when moving toward the critically constrained region, and quickly increases to almost a full size in the overconstrained region. The backbone of MAX 3-SAT with size 0.5 appears approximately at the location where 3-SAT is satisfiable with probability 0.5. Near this 0.5-0.5 phase transition collocation, the backbone of MAX 3-SAT and the satisfiability of 3-SAT seems to be linearly correlated.

This research makes two contributions. First, it reconciles the relationship between the phase transitions of decision and optimization problems, bridging the gap of the previous phase transition results on these two types of problems. Second, it suggests that backbone in the solutions of optimization problems is an order parameter for the problems.

This work also gives rise to many interesting open questions for future research. For instance, where is the exact phase transition location of bounded 3-SAT(B)? Why does the backbone of MAX 3-SAT with size 0.5 collocate with 50 percent satisfiability of 3-SAT? Why does the backbone appear to have a linear correlation with the satisfiability?

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