Behavior of heuristics and state space structure near SAT/UNSAT transition

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Abstract

We study the behavior of ASAT, a heuristic for solving satisfiability problems by stochastic local search near the SAT/UNSAT transition. The heuristic is focused, i.e. only variables in unsatisfied clauses are updated in each step, and is significantly simpler, while similar to, walksat or Focused Metropolis Search. We show that ASAT solves instances as large as \( N = 10^6 \) in linear time, on average, up to \( \alpha = 4.21 \) for random 3SAT. For \( K \) higher than 3, ASAT appears to solve instances at the Montanari-Ricci-Tersenghi-Parisi “FRSB threshold” \( \alpha_s(K) \) in linear time, up to \( K = 7 \).

1 Introduction

Satisfiability problems (SAT) appear critically in many disciplines. Finding fast and reliable numerical methods for solving them is crucial in industrial applications, such as scheduling, or in verification.

The random KSAT model, where each condition or clause has the same arity \( K \), and an instance is picked randomly, has been of interest both to theoretical computer science and to statistical physics. For \( K \geq 3 \) KSAT belongs to the NP complete class of problems. While a deterministic algorithm will always find a solution if there is one, it presumably takes a long time to solve a KSAT instance in worst case [1]. However, the typical behavior can be different. Indeed, since the beginning of the 90s it has been known that the average running time of a deterministic algorithm depends on \( \alpha = \frac{M}{N} \) the number of clauses \( (M) \) per variable \( (N) \) [2]. As \( \alpha \) varies, a SAT/UNSAT transition is observed at a critical value \( \alpha_{cr} \): below the threshold, a typical instance is satisfiable, while above \( \alpha_{cr} \) it is typically unsatisfiable. The transition becomes sharper as \( N \) increases [3]. Deterministic algorithms have (empirically) longest average run times close to \( \alpha_{cr} \) [2, 3, 4].

Stochastic search heuristics are not guaranteed to find a solution, if there is one, but may on the other hand greatly outperform a deterministic algorithm on a typical (solvable) instance. As \( \alpha \) increases for given \( K \) and \( N \), the typical run-time of a given heuristic increases, eventually diverging, at the latest at \( \alpha_{cr} \). The most interesting behavior, if it can be established, is if for
some heuristic the typical run-time grows only linearly in $N$ for sufficiently small $\alpha$, and also if the distribution of run-times per variable gets more narrow as $N$ increases. If so, run-time per variable is a self-averaging quantity. We denote here the greatest such $\alpha$ for some heuristic $\alpha_{\text{lin}}$, the linear-time transition for that heuristic.

A benchmark stochastic search is Papadimitriou’s RandomWalksat [5]: in every step an unsatisfied clause is picked randomly, and then one random variable in that clause is flipped. For that algorithm, rate equations and direct simulations indicate that $\alpha_{\text{lin}}$ on 3SAT is approximately 2.7 [6, 7]. Furthermore, for simple heuristics, such as straight-forward guessing without backtracking, rate equations and direct simulations also show a nonzero $\alpha_{\text{lin}}$, albeit smaller [8].

A limitation of RandomWalksat is that it does not distinguish between which variable in a clause to flip, or if flipping one increases or decreases the number of unsatisfied clauses. The walksat [9] algorithm mixes RandomWalksat moves with greedy steps, by default in equal proportion. Walksat has been known to be quite powerful on SAT problems, but it was only shown quite recently to have a $\alpha_{\text{lin}}$ of 4.15 on 3SAT [10]. In contrast to RandomWalksat, rate equations have not been set up for walksat: the interleaving of random and greedy moves, and the additional “freebie” move in the Selman-Kautz-Cohen heuristic, makes that complicated. Alava, Orponen and Seitz showed that $\alpha_{\text{lin}}$ for walksat could be pushed to or beyond 4.20 by optimizing over the proportion of random and greedy moves [11]. Furthermore, these authors showed that two other algorithms, Focused Metropolis Search (FMS) and Focused Record-to-Record Travel can be optimized to also have an apparent $\alpha_{\text{lin}}$ around 4.20. FMS in particular is quite simple: a variable in an unsatisfied clause is flipped if that decreases the number of unsatisfied clauses, and otherwise flipped or not flipped by a probability exponential in that number. FMS does not have the freebie move of walksat, but is still of comparable efficiency.

In this contribution we will introduce and study a heuristic ASAT, for average SAT, which is arguably yet simpler than FMS. In ASAT a variable is flipped if this decreases the number of unsatisfied clauses, as in FMS, and then flipped with a constant probability if the number of unsatisfied clauses increases. ASAT is therefore sensitive to the widths of local minima, but not directly to the heights of the walls around local minima.

The relevance of these studies lies along the following lines. First, more powerful search heuristics have a practical interest. While we do no not present detailed comparisons in this paper, let us state that ASAT generally runs somewhat faster than optimized FMS, which in turn is somewhat faster than optimized walksat with the Selman-Kautz-Cohen heuristic. More importantly, since ASAT is simpler than FMS, which in turn is simpler than walksat, one might hope for a analytical treatment along the lines of [6, 7]. Second, from the theoretical side, it is of interest if $\alpha_{\text{lin}}$ for ASAT and other heuristics lie beyond 4.20 on random 3SAT, since that lies beyond two natural candidates for upper bounds on $\alpha_{\text{lin}}$, known respectively as $\alpha_d$ (which is around 3.92 for random 3SAT) and $\alpha_s$ (around 4.15).

The theoretical background of these two numbers $\alpha_d$ and $\alpha_s$ can be briefly described as follows. Within the cavity method, it has been shown that for low enough $\alpha$ the set of solutions is connected, while in the interval $[\alpha_d, \alpha_c]$ the set breaks up into “clusters” [12, 13]. This was recently rigorously confirmed for large enough $K$ [14, 15]. A satisfiability problem is equivalent to the problem of finding a zero-energy ground-state in a statistical mechanics model, where the “energy” is the number of unsatisfied clauses. In the UNSAT regime, where an instance is typically unsatisfiable, the ground-state energy is typically larger than zero. In the SAT regime, clusters of solutions are local minima, which are also global minima. If these are accompanied by a much larger number of clusters with non-zero energy, such clusters could act as traps to
local search heuristics. The number of clusters of local minima at given energy was computed by the cavity method for random 3SAT in \[12, 13\], and for higher \(K\) in \[16\], and does increase with energy. One possible conjecture, already falsified in \[10\], would hence be that \(\alpha_d\) is an upper bound on \(\alpha_{lin}\). For KSAT a further phase transition takes place at \(\alpha_s\), inside the interval \([\alpha_d, \alpha_{cr}]\), giving rise to a hierarchical structure of clusters \[17\]. For random 3SAT, \(\alpha_s\) is approximately 4.15.

It is not clear to the present authors what the relation, if any, should be between \(\alpha_s\) and \(\alpha_{lin}\). Given however that \(\alpha_{lin}\) for default walksat is larger than \(\alpha_d\) and very close to \(\alpha_s\), one might conjecture that \(\alpha_s\) be an upper bound on \(\alpha_{lin}\). The results of this paper and of \[11\] on the other hand indicate that \(\alpha_{lin}\) for optimized algorithms is substantially larger than \(\alpha_s\) for 3SAT. We show that run-time of ASAT is self-averaging at \(\alpha = 4.21\) on 3SAT up to instances of one million variables, while it is not self-averaging at \(\alpha = 4.25\). It is difficult to pin-point more precisely the transition point in this interval. It is even more difficult to compute the transition line of KSAT at \(K\) larger than 3 accurately, as the memory requirements per variable grow as \(K\alpha\). We present here data that at \(\alpha_s(K)\), as computed recently in \[16\], run-times of ASAT seem self-averaging up to \(K = 7\). The time course of a solution is another quantity interest. Below \(\alpha_{lin}\), ASAT solves an instance in linear time, similarly to RandomWalksat below its \(\alpha_{lin}\). Above \(\alpha_{lin}\), but of course on a satisfiable instance, i.e. below \(\alpha_{cr}\), ASAT typically solves an instance by a slow process, “sinking” through several plateaus. We show results from one such run, and we note that it appears to be different from the “solution by fluctuations” proposed for RandomWalksat above its \(\alpha_{lin}\) \[6\]. To optimize ASAT we introduce a re-heating procedure, which also sheds light on the effective landscape seen by the algorithm.

2 The ASAT heuristic

ASAT is a focused heuristic, like RandomWalksat, walksat and FMS, meaning it focuses on the unsatisfied clauses at any given time, and makes a trial moves only to neighboring states by flipping a variable that appears in at least one unsatisfied clause. Variables that only appear in satisfied clauses are never flipped. In a sense, ASAT is perhaps the simplest extension of RandomWalksat. For any trial move, it only computes if that move will increase or decrease the energy (number of unsatisfied clauses). A move which increases the energy will be accepted with fixed probability, independent on how much the energy is changed, while a move that decrease the energy will be accepted always. In pseudo-code, ASAT is hence

\[
\text{s = initial random configuration}
\]

\[
\text{while } t < t_{\text{max}}
\]

\[
\text{if } F(s) = \text{TRUE then EXIT}
\]

\[
\text{at random pick a unsatisfied clause C}
\]

\[
\text{at random pick a variable x in C}
\]

\[
x' = \text{flip(x)}
\]

\[
s' = s(x \rightarrow x')
\]

\[
\text{if } E(s') \leq E(s) \text{ then flip x else}
\]

\[
\text{flip x with probability p}
\]
Figure 1: Ranked logarithmic run-times per variable of ASAT, $p = 0.21$, at $\alpha = 4.21$ and values of $N$ from $10^4$ to $10^6$ on 3SAT. Note pivoting of the distributions, as in [10]. Note that all runs were made with a cut-off of $5 \cdot 10^6 N$ flips. Out of one hundred, all instances at $N$ equal to $10^5$ and $10^6$ are solved within this time, most instances at $N = 10^6$ taking close to $10^{10}$ flips. For the smallest size, $N = 10^4$, the spread is larger, and about 10% of the instances are not solved in $5 \cdot 10^{10}$ flips, although the median is but a little more than $10^8$ flips.

The ASAT algorithm is therefore characterized by the single parameter $p$, which plays an analogous role to the proportion of random and greedy moves in walksat (a parameter also called $p$), and the noise parameter $\eta$ of FMS. Optimization of $p$ in ASAT is discussed below in section 3. Fig. 1 shows a rank ordered plot of the run-times for different system sizes $N = 10^4, 10^5, 10^6$ at $\alpha = 4.21$. This and analogous data for several lower values of $\alpha$ (data not shown) indicate that the run-time of ASAT is self-averaging at least this far.

As an example of lack of self-averaging, we show in Fig. 2 a rank ordered plot at $\alpha = 4.25$, the conjectured end point of the SID (Survey Induced Decimation) algorithm [13, 12]. Clearly here there is no sign of self-averaging.

The plot in Fig. 1 is in a sense misleading, as there are finite-size effects at smaller $N$. In other words, “good pivoting” and hence (numerically) convincing self-averaging is only displayed from values of $N$ around $10^4$ and upwards. Similar finite-size effects were noted by the authors of [11] on optimized FMS (data unpublished) and by one of us on walksat, and are presumably a feature of the constant-$\alpha$ ensemble. It seems that the onset of good pivoting increases with $\alpha$, which makes a precise determination of $\alpha_{lin}$ difficult. The largest instances that fit into memory of
Figure 2: Ranked logarithmic run-times per variable of ASAT, $p = 0.21$, at $\alpha = 4.25$ and values of $N$ from $10^4$ to $10^6$ on 3SAT.

Present generation workstations is on the order of a million variables at $\alpha \sim \alpha_{cr}$: there are $\alpha N$ clauses, each one of them specified by $K$ integers, which for $K = 3$ and $\alpha \sim 4$ makes about $50 \cdot N$ bytes. Hence, for $\alpha$ larger than 4.21 the interval between the onset of good pivoting and the largest instances that can be investigated is too small to draw a conclusion. For higher values $K$ the problem quickly becomes worse, since $\alpha_{cr}$ increases, roughly as $2^K$.

The solution process can be characterized by the fraction of unsatisfied clauses as a function of the number of flips. Following [6, 7, 8] it is convenient to introduce a “time” as $\text{flips}/N$. Fig. 3 shows the time course of a solution process at $\alpha = 4.22$. One can clearly see three regimes, one fast, one intermediate, and one quite slow. The fast regime, up to time about ten thousand, is presumably analogous to the Poissonian regime in RandomWalksat as studied by [6, 7]. The intermediate and slow regimes have, as far as we know, not been shown on this problem previously. We note that dynamics appears self-averaging in both the fast and the intermediate regime; perhaps hence both the fast and the intermediate regimes will be amenable to analysis. The slow regime proceeds by plateaus (long waiting periods). While this qualitative behavior repeats itself from run to run, the position and lengths of the plateaus do not. In the slow regime, dynamics is hence not self-averaging. We note that this solution mode, “slowly sinking in the energy landscape”, seems qualitatively different from the “solution by fluctuations” found for RandomWalksat in [6, 7].

Finally, we have investigated ASAT for $K$ larger than 3, albeit in less detail. While computational determination of the threshold gets harder at higher values of $K$, one may look for evidence that some given $\alpha$ is comfortably below $\alpha_{lin}$. In Fig. 4 we have looked at $\alpha_s(K)$, which
Figure 3: Time course of solution of one instance by ASAT at $\alpha = 4.22$ and $N = 10^6$. Note that ASAT solves this instance, but only after $1.3 \times 10^5$ time steps, i.e. $1.3 \times 10^{11}$ flips. The main plot, in logarithmic coordinates, shows that the solution proceeds in three stages. First, there is decay on a time scale up to about $10^3$. This process slows down, and is overtaken another process which last up to time about $2 \times 10^4$. Finally, there is a very slow decrease to the solution. Top insert shows a blow-up of the second stage in linear coordinates. Bottom insert shows the final decrease, which proceeds by plateaus, where the energy is approximately constant. In this run three plateaus can be discerned, with, approximately, 200, 50 and 15 unsatisfied variables, respectively.
Figure 4: Median and quartile run times per variable at $\alpha = \alpha_s(K)$, values taken from [16]. Figure indicates that ASAT solves these instances with about equal computational cost per variable, for all $K$. The parameter $p$ was found by procedure ASAT-HEAT (see main text) on each value of $K$ separately. The values were 0.21, 0.118, 0.068, 0.045 and 0.032 for $K$ from 3 to 7, respectively.

The results are not entirely conclusive, but tend to support that $\alpha_{lin}$ is greater than $\alpha_s$.

3 State space structure and parameter optimization

In this section we describe a method to optimize the value of the noise parameter $p$. The method called simulated heating of ASAT, or ASAT-HEAT, is also, as we will see, a useful tool when investigating the local barriers of random K-SAT.

The idea is that there is a trade-off to be made between an algorithm getting out of local minima, and efficiently exploring the bottom of a local minimum. Hence, the premise is that solutions are found at the bottom of some local minima, which are not otherwise distinguished. After completion of this work, we became aware of a related idea, "optimization at the ergodic
edge”, has recently been considered by Boettcher and Frank [18], and also, to optimize the Record-to-Record-Travel algorithm, by Jia, Moore and Selman [19].

In the context of ASAT we look for the value $p$ such that the algorithm does not get stuck, while still exploring the bottom of minima where it finds itself. That is done by an interleaved process, where the algorithm alternatively runs with some non-zero $p$ (to explore phase space, and get out of minima), and alternatively freezes at zero $p$ (to find the bottom of the minimum it is moving in). In ASAT-HEAT the value of $p$ is raised incrementally in the following steps:

- Generate an problem instance of size $N$ close to $\alpha_{cr}$.
- Run the heuristic with a low value of the parameter $p$ and let the system equilibrate for some time $\tau >> 1$. We have used $\tau$ equal to one thousand, i.e. $10^3 N$ flips.
- Do a zero temperature quench, that is set the noise parameter to zero. The heuristic will then find a near local optimum by greedy search.
- Reset the parameter $p$ to its previous value, increase it by a small amount $\Delta p$, and let the system again equilibrate for a time $\tau$.
- Iterate heating and quench.

Fig. 5 shows ASAT-HEAT for a system at $K = 3$, $N = 10^4$ and $\alpha = \alpha_{c} = 4.27$. Up to $p_{cr} \sim 0.21$ the variations during the heating periods increase with $p$, while the lowest energies reached after the zero-temperature quench trend downward. Furthermore, the lowest energies seen during the heating periods are quite similar to the lowest energies after quench. This suggests that the algorithm is here in contact with the local structure, i.e. that the algorithm visits the local minima also during the heating periods. The downward trend of the lowest energies after quench indicates that the algorithm over time explores a larger set of minima, reaching lower energies, compare the time course of a simulation as in Fig. 8.

After $p_{cr} \sim 0.21$, the variations during the heating periods are larger. The energies reached after quench are clearly lower than the ranges seen during the heating periods, indicating that the algorithm has now lost contact with the local structure. The energies reached after quench on the other hand increase with $p$, indicating that the algorithm now moves in higher-lying and more numerous local minima. We have found that ASAT works most efficiently using values of $p$ at or slightly above $p_{cr}$.

To investigate how the algorithm moves in state space, we compute the Hamming distance between the state at some time (some value of $p$ in ASAT-HEAT), and a reference state at the initial value of $p$. Fig. 6 shows the variation in Hamming distance for system size $N = 10^4$, which exhibits a step-wise increase by plateaus. Fluctuations in Hamming distance are small below $p_{cr}$, and increase rapidly above $p_{cr}$.

We have further investigated how $p_{cr}$ varies with $N$ by running simulations at ten times the original system size. The overall behavior is similar and the transition seems to take place at or close to the same value of $p$. This suggests that the local small scale structure does not depend or depends only weakly on $N$. The value of $p_{cr}$ found by ASAT-HEAT decreases with $K$; the values for $K$ from 3 to 7 are given in caption to Fig. 8.
Figure 5: Escape from meta-stable state at $\alpha = 4.27$ and $N = 10^4$ while increasing parameter $p$ in procedure ASAT-HEAT (see main text). Note that up to a critical value $p_{cr}$ fluctuations are small and the energy decreases slowly. At higher values of $p$, fluctuations are larger, and energy increases with $p$. Figure shows every $N$th time point during the heating periods ($p$ greater than zero) and the zero-temperature quenches, at each value of $p$, respectively.
Figure 6: Same run as in Fig. 5. Hamming distance from initial meta-stable state increases with $p$ by plateaus up to the critical value, at which it remains stationary. Fluctuations are relatively larger above the critical $p$.

4 Discussion

We have in this work presented a new heuristic for satisfiability problems, called ASAT. The heuristic has been implemented as an additional option in walksat (walksat distribution format [20]), and is available upon request. One main interest of ASAT is that it is competitive with walksat and Focused Metropolis Search (FMS) on random $K$ SAT problems close to the SAT/UNSAT transition, while being simpler, and hence (hopefully) amenable to analytic investigations. We hope to return to this question in a future contribution.

We have shown that ASAT has typical runtime linear in $N$ up to $\alpha = 4.21$ on 3SAT, up to the largest instances that can be studied ($N \sim 10^6$). We can not exclude that ASAT will eventually not look linear on even higher values of $N$, but we see no sign of such divergence. Finite-size effects make it difficult to show if or if not ASAT is linear or not beyond $\alpha = 4.21$. This means, that to the best of our estimate, the linearity threshold for ASAT, $\alpha_{lin}$, is for random, 3SAT larger than both the clustering transition ($\alpha_d = 3.92$) and the “FRSB threshold” ($\alpha_s = 4.15$). We have studied ASAT at larger $K$, and showed that probably $\alpha_{lin}$ is likely to be larger than $\alpha_s$ there also.

A parameter optimization technique, ASAT-HEAT, has been introduced. This allows for a determination of an optimal parameter value of the algorithm, and can be considered an alternative to the extensive simulations at many values of $N$, $\alpha$ and one algorithm parameter used in [11].

While physical intuition suggests that local heuristics will have difficulties where many meta-stable states appear (at $\alpha_d$, or perhaps, more properly, at $\alpha_s$) this does not seem to be the case.
RandomWalksat and very simple heuristics have difficulties far below $\alpha_d$, while ASAT and other heuristics seem to work linearly beyond $\alpha_s$. Let us therefore end by stating the differences between stochastic local search heuristics to find satisfying assignments in random KSAT and a physical process of random walk in a corresponding energy landscape. First, RandomWalksat, walksat, FMS and ASAT are focused: these algorithms correspond to non-equilibrium dynamics without detailed balance \cite{7}. Conservation of any cluster structure at all under non-equilibrium perturbations has apparently been a moot point in some spin glass models \cite{21, 22}. Second, while FMS is similar to a random walk in the energy landscape, in the sense that the dynamics directly depends on the local energy, walksat and ASAT and obviously RandomWalksat do not. In walksat with Selman-Kautz-Cohen heuristic, decisions are based on the change in “breakclause” which is not the same as the energy change, while in ASAT decisions are based on whether the energy increases or decreases at all. Therefore, finally, while numerical simulations cannot rule out that e.g. ASAT will run into trouble beyond $\alpha_s$ on instances larger than the ones we have studied, we are not sure if it necessarily has to. Theoretical predictions on what $N$ one would expect to see nonlinear behavior at what $\alpha$ would be most helpful to guide numerical experiments on this issue.

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