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On Dynamic Phase Transitions in Satisfiability Problems

John Ardelius

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Abstract

The problems to optimize properties of a frustrated system of many variables is a complex matter. Such problems arise in both combinatorial computational problems as well as in complex materials such as spin glasses.

Since the theoretical treatment of such system is very hard and complicated one would like to find simpler methods to examine them.

In this thesis random K-SAT problems are studied. We have developed a new heuristic method called ASAT which is a stochastic local search method which seem to be faster and simpler than existing ones. It is able to solve problem instances in linear time up to the constraint per variable ratio 4.21.

We also examine the state space structure seen by the heuristic by a procedure called 'Simulated heating'. This also reveals the optimal value for the noise parameter in the optimization problem. How this scale with constraint size, K, is also investigated.

Finally we use a statistic approach and model random 3-SAT problems with master equations.

Keywords: Random K-SAT, Stochastic Local Search, ASAT, Frustration, Dynamic Phase Transition, Simulated Heating, State Space Structure, Multivariate Optimization

Contents

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Chapter 1

Introduction

For sometime now theories from statistical physics have been used to solve computational problems in computer science. Many hard computation/optimization problems bear close resemblance with physical systems in the sense that they both contain a large number of degrees of freedom.

Some twenty years ago the connection between physical and computational models became even more apparent when a class of problems known as satisfiability problems (SAT) displayed a first order phase transition [1]. The system changes from being in general easy solvable to in general very hard to solve at a distinct value of a system specific order parameter.

To find these physical behaviors in computational problems have raised the question of weather or not the nature of computational complexity and other properties may be explained in traditional physical terms.

The main problem in optimizing systems with many degrees of freedom is that any algorithmic strategies based on global knowledge will grow extensively with system size, resulting in a computational cost that vastly exceeds the capacity of the fastest computer!

One successful approach to this problem come from the theoretical treatment of a class of complex physical systems called binary magnetic alloys or *spin glasses*. Spin glass materials are class of systems which display *frustration*. Frustration in this context means that there are many conflicting interactions that will affect the system on its way towards equilibrium. Therefor the dynamics of the process affects properties of the system itself, making detailed structure hard to predict. The same is true for a computational model called the *SAT model*. In the past few years a lot of effort has been made to understand the statistical as well as dynamical properties of spin glasses as well as SAT problems. This theory has resulted in actual solving algorithms for computational problems which have shown to be very effective.

Another strategy have been to use local properties of the system to guide an iterative random optimization algorithm through the system state space eventually reaching an optimal configuration. This approach is called stochastic local search, SLS. Recently SLS heuristics have shown to be surprisingly successful in finding optimal configurations in hard SAT problems [2]. Despite their simplicity and inherent stochastic nature, they have shown to be competitive to the more theoretically based ones and whether or not they are just as good is still an open question.

To examine why and how these local heuristics are so successful is the main part of this thesis. This area of science where problems from traditional physics and information theory show apparent similarities is a interesting and active area which will hopefully lead to many insights regarding the very nature of complex systems.

The thesis is organized as follows. Chapter 2 contains a brief overview of traditional statistical mechanics as well as complexity classes in computer science. The SAT model is introduced. Chapter 3 outlines the current status of the field and the issues that are being treated. In Chapter 4 a new heuristic for solving random K-SAT problems is introduced and compared to existing ones. It is used in Chapter 5 to examine the complex state space of SAT problems. An analytical approach using master equations is described in Chapter 6. The thesis ends with a conclusion and a future outlook of the field.

1.1 Main results

Some of the results presented in the thesis are:

- The new heuristic, ASAT, is faster than existing ones in terms of finding a solution in number of iterations/system size.
- The dynamics of the process, close to the SAT/UNSAT transition, seems to display different behavior on different timescales. Similar to the *aging* process in spin glasses.
- The metastable states where the heuristic is trapped seem to be of two kinds; one where the temperature (noise parameter) is simply too high to let the system get trapped in any small scale structure, and one where it is trapped, a *trapping state*.
- The critical temperature where the system is able to leave a trapping state seems to be invariant in system size and shows resemblance to the *glass temperature* T_g in spin glasses.

Chapter 2

Theoretical background

In this chapter some essential theory is briefly described from various fields as complexity theory and statistical mechanics and some key concepts are defined. The introduction will not be comprehensive and some background knowledge in physics is assumed. Last the SAT model is introduced which is the central model used throughout the thesis.

2.1 Computational problems

In theoretical computer science one divides computational problems in complexity classes depending on how the solution time depends on system size (N) for an average instance of the problem. Somewhat simplified the main classes are;

P, which consists of problem solvable in time polynomial in N, i.e. there exists deterministic algorithms for finding the solutions.

NP, which consists of problem for which no known deterministic algorithm exist but if one finds a solution, it can be verified in polynomial time.

NP-C or "NP complete" are the problems that are at least as hard as any NP problem and any other problem in this class can be reduced to it. There are a lot of more or less classical NP-complete problems [3] and an efficient algorithm for solving one of them would be able to solve them all.

There are however another approach to treat NP-C problems. The use of algorithms which are not proved to work deterministic but often finds a "good enough" solution in many cases are called *heuristics*. Finding good heuristics is an important part of designing practical applications.

A large part of the NP-C problems are so called combinatorial optimization (CO) problems. The task in CO is to combine the elements of a system in such a way that some property

of the system, as a whole, is optimized. This might be to connect points on a lattice to minimize the total distance (traveling salesman, TSP) or minimizing the energy of interacting particles in a compound.

2.2 Statistical mechanics

2.2.1 Equilibrium distribution

The idea behind statistical thermodynamics is that the properties of a macroscopic system can be derived from statistical calculations on its microscopic structure. The number of possible ways to arrange a microscopic system is denoted W. From this one can calculate the macroscopic entropy (and other properties) of the system through Boltzmann's classical formula

$$S = k_B ln(W) \tag{2.1}$$

Instead of computing W one can use the probability distribution of the microscopic states (s in number) which yields [see e.g. [4]]:

$$S = -k_B \sum_{i=1}^{s} p_i ln(p_i) \tag{2.2}$$

According to the second law of thermodynamics the entropy will, at equilibrium, tend to a maximum. Therefore one can regard the equilibrium system as a optimization problem to find the probabilities p_i which maximizes the entropy.

In many cases there are constraints on the system e.g. conservation of energy $< H(x) >= E$ or any constraint function $g(x)$. (x are the generalized coordinates of the system). Together with the condition $\sum_{i=1}^{s} p_i = 1$ the problem to solve is:
maximize

$$S(p) = -k_B \sum_{i=1}^{s} p_i ln(p_i) \tag{2.3}$$

subject to

$$g_1(p) = \sum_{i=1}^{s} p_i = 1 \tag{2.4}$$

and

$$g_2(p) = \sum_{i=1}^{s} p_i E_i = \text{Ç} \tag{2.5}$$

This is easily solved by use of Lagrange multipliers (see e.g. [5] for details on optimization).

$$(\frac{\delta S}{\delta p_i}) - \lambda_1(\frac{\delta g_1}{\delta p_i}) - \lambda_2(\frac{\delta g_2}{\delta p_i}) = 0; i = 1..s \Rightarrow \tag{2.6}$$

$$\Rightarrow -1 - k_B ln(p_i) - \lambda_1 - \lambda_2 E_i = 0 \Rightarrow \tag{2.7}$$

$$\Rightarrow p_i = e^{(-1-\lambda_1-\lambda_2 E_i)/k_B} \tag{2.8}$$

Normalizing this gives:

$$p_i = \frac{p_i}{\sum_{j=1}^{s} p_j} = \frac{e^{(-\lambda_2 E_i)/k_B}}{\sum_{j=1}^{s} e^{(-\lambda_2 E_j)/k_B}} \tag{2.9}$$

If E_j is the energy of the state (which it often is) the multiplier λ_2 will turn out to be the inverse temperature of the system. The entity $1/k_B T$ is often denoted β.

The properties of the macroscopic system can now be calculated through the partition function $Z = \sum_{j=1}^{s} e^{-\beta E_j}$. The quantity $e^{-\beta E_i}$ is, when normalized, the probability density for the system to be in a state with energy (or any other constrained parameter value) E_i. Any equilibrium property of the system can be calculated statistically as the ensemble average

$$< A >= \sum_{j=1}^{s} A_j p_j = \frac{\sum_{j=1}^{s} A_i e^{-\beta E_j}}{Z} \tag{2.10}$$

One should remember that this distribution comes from the fact that the system is constrained. If there are no constraints the above calculations will give $p_i = 1/s$. That is, every state is equally probable.

2.2.2 Thermodynamical limits

As the system grows, the variance of the expectation values will decrease as $1/\sqrt{(N)}$ and values for physical macroscopic systems ($N_a \propto 10^{23}$) will be very well defined. The limit when systemsize(N) and system volume (V) tend to infinity keeping the ratio N/V constant is called the *thermodynamical limit*. Properties that become well defined in this limit are called *self averaging*. Almost all thermodynamical calculations are done in this limit.

At *equilibrium*, that is $t \to \infty$, all transient behavior of the system will be gone and all expectation values will be time independent.

Another important thermodynamic limit is the *zero temperature limit*. When temperature decreases the partionfunction approaches $Z_0 = \sum_{j=1}^{s_0} e^{-\beta E_0}$. The s_0 states with energy E_0 are called the systems *ground states*. All other states will appear with probability $p_i \to 0$ as $T \to 0$.

2.2.3 Frustrated systems

Many physical systems are modeled as a grid or discrete lattice in a normal (n-dimensional) Euclidean space. On each lattice point sits some entity which can be seen as a stochastic variable. Such systems are generally referred to as a *random field*. Examples of random fields are the famous Ising model or the SAT model (see below).
The interactions between the lattice sites in the field are modeled using some energy function

$$H(x_i) = \sum_{i=1}^{N} f(x_i) + \sum_{i,j=1}^{N} g(x_i, x_j) \tag{2.11}$$

The problem is then to minimize the energy with respect to the values of the random variables x_i.

Sometimes several contradicting interactions affect a variable and there is no unique value it can have to minimize all interactions. The variable is then said to be *frustrated*.

As an example of a frustrated system lets say that every particle is a person with a certain opinion on a matter. If the matter is controversial then interaction with people with other opinions might be difficult. To minimize conflicts (energy) the person will probably group with people that share his/her view.

On the other hand if the matter is of no importance, meeting people with other opinions will be no problem. In the border between the two scenarios (phases in physics) there might be many different group constellations and it is not obvious which one will minimize conflicts.
Example of frustrated systems in physics are e.g. spin glass materials and the SAT model (see below).

2.3 The SAT model

Satisfiability is a theoretical problem in which one is to find out whether or not a certain logical statement is true or false. Given a binary string of N variables (truth assignment) and M conditions on the variables, is it possible to flip the value of the variables so that all M conditions are fulfilled? In practical applications one typically has some specific constraint on the variables whereas here the constraints are generated at random. For instance all references in the thesis to SAT problems means *random K-SAT*.

To construct a SAT problem (problem instance) one first generates a random binary string of length N. Then K out of the N variables are randomly picked and negated with 50% probability. A variable and its sign is denoted a *literal*. The logical disjunction of the K literals is called a *clause* and M such clauses are constructed. For the instance to be

satisfied all of the M clauses have to be evaluated to true.

In mathematical notation, one constructs a truth assignment where 1=TRUE and 0=FALSE.

$$S = \{s_i = 0, 1\}_{i=1,..,N} \tag{2.12}$$

Then one constructs K literals,

$$\{x_k = \{s_1, s_2, .., s_N, \neg s_1, \neg s_2, .., \neg s_N\}_{k=1,..,K} \tag{2.13}$$

and M clauses are formed by disjunction of the literals.

$$C_j = (x_1 \vee x_2 \vee x_3 ... \vee x_K)_{j=1,..,M} \tag{2.14}$$

A conjunction of all clauses forms the formula which is to be satisfied:

$$F = \{s_i = 0, 1\}_{i=1,..,N} \tag{2.15}$$

As an example a construction of a SAT problem with N=5, K=3 and M=4 will be done like this: The initial assignment are N=5 random binary variables say $s_1 = 0$, $s_2 = 1$, $s_3 = 1$, $s_4 = 0$ and $s_5 = 1$. Pick K=3 of them and negate with equal probability. This will perhaps be $x_1 = s_3$, $x_2 = \neg s_1$ and $x_3 = \neg s_5$. Put logical OR between the literals and do this M=3 times:
$C_1 = (s_3 \vee \neg s_1 \vee \neg s_5)$; $C_2 = (s_1 \vee s_5 \vee \neg s_2)$; $C_3 = (\neg s_3 \vee \neg s_2 \vee s_4)$.

The initial value for the first clause will be: $(1 \vee \neg 0 \vee \neg 1)$ There is only one false assignment in this clause namely $\neg 1$ = NOT TRUE = FALSE. The rest of the assignments are correct however and the clause as a whole will be evaluated to TRUE. The same is true for the second clause but the third will evaluate to $(\neg 1 \vee \neg 1 \vee 0)$ = (NOT TRUE) OR (NOT TRUE) OR (FALSE) = FALSE. For the formula to be satisfied all three clauses has to be satisfied so the initial formula is currently unsatisfied. Flipping literal s_3 from 1 to 0 will make the third clause satisfied without turning any other clause unsatisfied. A satisfying assignment is therefore $S^* = \{0, 1, 0, 0, 1\}$.

This may look easy, but as soon as the number of variables and clauses grow finding satisfying assignments is far from trivial. In fact for $K >= 3$ the problem of finding a solution was one of the first problems shown to be NP complete.

In the context of SAT problems one also defines a complexity parameter $\alpha = \frac{M}{N}$ which indicates how many constraints there are, on average, on each variable. Another notation

that will be used is that if a variable is the sole satisfying variable in a clause it is said to be of type *S1T*. If there are two satisfying variables they are of type *S2T* and so forth.

2.3.1 Graph theoretical view on SAT

A SAT problem can also be modeled as a network where the nodes are clauses and variables respectively. Clauses are denoted with squares whereas variables with circles. Two variables are said to be *neighbors* if they both are involved in some constraint i.e. contained in the same clause. An example of a 3-SAT problem may then look like below.

The view is also useful in modeling *loops* in the dynamics. Loops in this context are flipping sequences that at the same rate as they remove unsatisfied clauses create new ones. There are suggestions [2] that it is the onset of loops with extensive, $O(N)$, size that are responsible for the metastable states.

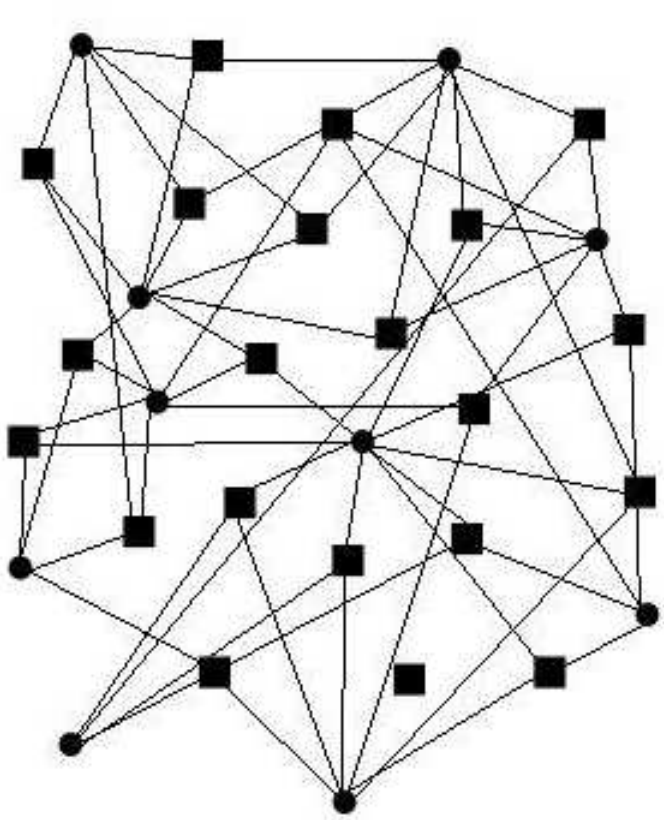

Figure 2.1: Shematic picture of K-SAT graph. Clauses are modeled as squares and variables as dots.

Chapter 3

Current status of the field

To get some perspective on the issues discussed in the thesis some background of important results in the field is presented briefly.

3.1 Simulated annealing

In 1983 Kirkpatrick et al. [6] published an article in Science that exploited the similarities between multivariate problems and statistical mechanics. The method used was called "Simulated Annealing".
The idea behind the technique is to first assign an energy or target function dependent on the configuration of the system parameters. E.g. the length of a trip around certain cites given the order in which they are visited, $L(\bar{x})$, is a property one would like to minimize.

The different configurations of the system thus result in different values of the target function and form an "energy landscape" in which one wants to find a minimum.

Annealing is a term from physics in which a system is cooled slowly in order to let it come to an equilibrium state without being trapped or quenched in a non ground state. The same idea can be applied to the optimization problem. One then first choose a configuration randomly and thus receive an initial energy $L_i(\bar{x})$. Then pick another configuration by changing one or a couple (not all) of variables and compute the new energy $L_f(\bar{x})$. If $L_f(\bar{x}) < L_i(\bar{x})$ accept the new configuration and if not accept is with probability $e^{\beta(L_i - L_f)}$. That is if the new configuration is better take it! otherwise accept it with a probability exponential in the difference in energy.

The parameter β thus affects the probability to move to a less favorable state and is analogous to the inverse temperature in a physical system. By increasing β one makes it

more improbable for the system to move up in energy. The risk is then to get trapped in a local optimal state. By slowly increasing the value of β (cooling the system) the system will eventually only be trapped in the lowest optimum i.e. the ground state.

The method has been successful in finding good or *nearly optimal* solutions in many problems but if the energy landscape contains a lot of deep local optimas the method will require unpractically long time.

3.2 Non equilibrium system

Simulated annealing and similar methods are equilibrium methods in the sense that optimal solution is expected to be reachable from every possible initial configuration. If the temperature is lowered slowly enough one will eventually find a ground state.
In more complex systems such as spin glasses or SAT problems the energy landscape can change with the energy or target function. As an analogy one can imagine a critical value of the energy (or temperature) T_c which determines the shape of the energy landscape [7]. Above T_c a single optimum is present whereas below there might be many. How and at what parameter values these effect appear is a complicated matter and lot of research is currently being done in this area.

Another problem with equilibrium methods is that it might not even be possible to move from one initial state to an optimum without changing all or a large fraction of the variables. This property is known as *clustering* of the solutions in phase space. Any method that only moves locally will only find a solution if its initial configuration is within a cluster that contains a ground state.
Some difficulties in treating non equilibrium systems theoretically comes from the fact that the condition of detailed balance does not necessarily hold. It is formulated as:

$$w_{ij}p_j = w_{ji}p_i \tag{3.1}$$

for all states i and j. w_{ij} is the transition rate to move from state i to state j. And p_i is the probability to be in state i. This condition is only valid, of course, when the system is in equilibrium. Symmetries of this kind is often exploited in equilibrium methods.

3.3 Random K-SAT

The physical community started to show interest in SAT problems when in 1994 [1] Kirkpatrick et.al showed that random K-SAT displays a first order phase transition. A first order transition is characterized by a noncontinuous change in some system specific order parameter.

In the case of random K-SAT the parameter is α (the ration of clauses to variables). Below the threshold, α_c, the system is for any instance of the problem in general easy to solve (to find a satisfying configuration). Above α_c on the other hand a general instance of random K-SAT appeared to be very hard, or impossible, to solve. The critical value of α was found to be more well defined with increasing system size i.e. in the thermodynamical limit the suggestion was that a distinct border between a "easy" and "hard" region was found.

3.3.1 Analytical approaches

As mentioned above the random K-SAT model have similarities to diluted spin glass models. Spin glasses and other amorphous materials is active area of research among theoretical physicists and a lot of effort have been made to understand the dynamics of such systems. To mention a few of the methods from statistical mechanics that are used in SAT context the *replica approach* have been very successful in predicting the critical value α_c as well as the *cavity field method*. The description of these methods are beyond the scope of this thesis. An introduction to them can be found in [8].

By use of the such theoretical analysis Mezard et al [9] constructed, in 2002, a very efficient algorithm called *survey propagation*. Survey propagation is able to solve instances above $\alpha = 4.25$ which is very close to the critical value. This is so far the best known algorithm.

Another important result from the theoretical analysis is that existence of a second phase transition. This transition is in the SAT phase and marks the onset of *clustering* of state space. This means that above this transition, if different solutions can be reached by flipping single variables in the instance they belong to the same cluster. The clusters are separated by some kind of barrier which is the number of variables one needs to flip to move from a solution in one cluster to a solution in another. The critical value of $\alpha = \alpha_d$ known as the *clustering transition* is known to be about 3.9 [10].

The dynamic nature of these cluster barriers is not rigorously investigated. One assumption is that the height of the barrier in terms of energy will scale as some polynomial in system size $P(N)$. If this is the case then any SLS approach will with certainty fail in the thermodynamical limit, no matter how high the noise parameter is set, it will not be enough to escape the local optimas [11].

3.3.2 Heuristic approach

As mentioned above one would ideally like to have a fast deterministic algorithm which where guarantied to solve any problem instance. For complex problems such as hard SAT

problems this is not possible. Although methods such as survey propagation are very successful so are many simpler methods. These methods are denoted *heuristics* instead of algorithms, as they are not deterministic in finding solution. A broader notation is *stochastic local search* (SLS) methods. These methods makes use of local information about a certain state and where to move is decided by some simple rule along with some inherent randomness. The advantage of SLS is that one does not need to have any global knowledge of the system as a whole if one only knows the status of the current state. The process is then Markovian in the sense that the value of the next state only depends on the previous, not on the whole process.

On random K-SAT one of the first such heuristics was a procedure made by Papadimitrou [12]. The pseudo code for this heuristic looks like this:

```
s = initial random configuration

while t<t_max
       if F(s) = TRUE then EXIT
       at random pick a unsatisfied clause C

       */
       at random pick one such variable x in C
       /*

       x' = flip(x)
       s' = s(x -> x')
```

An extension to this was *WalkSAT* [23] which makes use of a little bit more information:

```
       */
       if some variable in C can be flipped
       without breaking any clauses then
           at random pick one such variable x in C
       else
           -with probability p pick a random variable x in C
           -with probability (1-p) pick a variable x in C
            that breaks a minimal number of clauses
       /*
```

The main reason for the success of these heuristics is that they only focuses on the clauses yet to be satisfied. Why this approach works so well is not yet fully understood and one would like to make some analytic analysis of the behavior of the behavior. This is difficult because of the number of choices the heuristic makes use of. In each step one will have to

consider many different options and thus makes a theoretical analysis hard.

On statistical approach to random K-SAT was done by Barthel et al [13] in 2003. They considered the probability that a variable belongs to a certain number of satisfied and unsatisfied clauses respectively denoted $p(u, s)$. They then formulated a set of differential equations (master equation) for the probabilities that a variable changes according to the rules of the heuristic. The result was in good agreement with numerical results and another approach along this line will be presented in ch.6.

Recently a new heuristic called *Focused metropolis search* (FMS) was introduced [2].

```
s = initial random configuration

while t<t_max
       if F(s) = TRUE then EXIT
       at random pick a unsatisfied clause C
       at random pick a variable x in C

       x' = flip(x)
       s' = s(x -> x')

       if E(s') <= E(s) then flip x else
              flip x with probability C*exp(E(s')-E(s))
```

The properties of FMS is discussed in section 4.1.

Each heuristic has its own value for the critical value of α which is the highest value for which the heuristic is able to solve an average instance. This is denoted the *dynamic* transition value α_d. The value of α_d is thus a property of the details of the dynamics as well as the problem instance.

Chapter 4

ASAT - A new heuristic

In this chapter a new heuristic, ASAT, is introduced and properties of it compared to existing ones are discussed.

4.1 Extended FMS

The first task in this diploma work was to confirm the new found property of FMS i.e. that the computation time is linear in systemsize for an average instance of random 3-SAT for α very close to α_c.
To show this 100 instances was generated at N = 1000, 2000 and 4000 for $\alpha = 4.21$. A rank plot for the solution time for each of these instances is plotted in fig 4.1. As can be

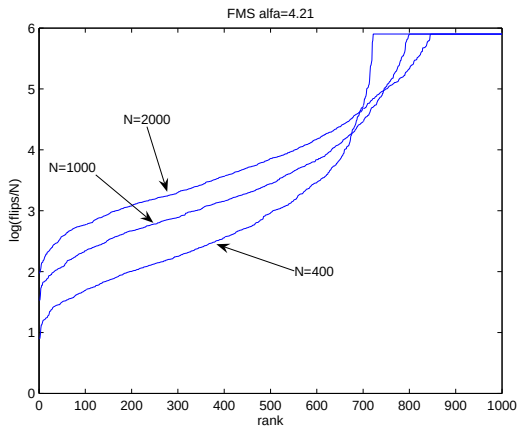

Figure 4.1: Run-times for FMS N=400,1000,2000 alpha=4.21.

seen the curves pivot around a certain point and more and more instances are solved as N increases. This *pivoting property* is a sign of self averaging of the run-times. That is when

$N \to \infty$ one would expect the the values to be very well defined. This is of course not a rigorous proof but contradict the existing theoretical belief that local heuristics will face severe problems even for $\alpha < 4$.

As FMS makes use of the energy difference between states as a guide through state space an idea would be to extend the energy function to include other properties of the states such as the number of neighbors of a trial state, s' or such. The approach here is to include the number of S1T neighbors of the trial state (see chapter 2) in the energy function. The reason is that it is only the S1T clauses that can turn in to UNSAT clauses. If one therefore introduces some bias to avoid clauses with a tendency to increase the number of UNSAT clauses (many S1T neighbors) the dynamics might be altered in some way.

$$H_{FMS} = E(s') - E(s) \tag{4.1}$$

$$H_{FMS+} = E(s') - E(s) + B * S1T(s') \tag{4.2}$$

The result of this ansatz did not turn out to be any different from FMS. This may indicate that the dynamics is too complex to be modeled on a time scale $\tau \propto O(t_{flip})$, where t_{flip} is a single flip of one of the N variables. One may have to look at the averages over times $\tau \propto O(N * t_{flip})$ to be able to capture some interesting behavior.

4.2 Clause correlations

Even though the ideas above for *extended FMS* did not seem to be fruitful, there might be time correlations in the number of a certain type (e.g. S1T) of clauses. That such *buildups* of correlations among certain clauses exists is suggested in [13]. To examine whether or not there are such correlations a simulations is run and in each time step the number of S1 neighbors of U clauses is compared to the average value if they where randomly distributed. The number of U-S1 neighbors, if there are no correlations, denoted $(U, S1)$ is:

$$(U, S1) = U * \frac{S_1}{\sum_i S_i} * 3 * 3\alpha = 9 * \frac{U * S_1}{N} \tag{4.3}$$

where U is the number of UNSAT clauses and S_i the number of clauses satisfied by i variables. There are 3 configuration that gives a S1T clause. Each clause has on average 3α neighbors. In a simulation with $N = 10^4$ and $\alpha = 4.2$ the above calculations was carried out in each time step and was subtracted from the actual number of U-S1 neighbors.

The result shows that the actual value is close to the "random" value. It seems normal distributed around zero. According to this one might suggest that this is the reason FMS+ did not work out. The dynamics does not seem to depend on the number of S1T neighbors on short timescales.
Another plot,fig 4.3, of the fraction of U,S1,S2 and S3 clauses also shows that after a

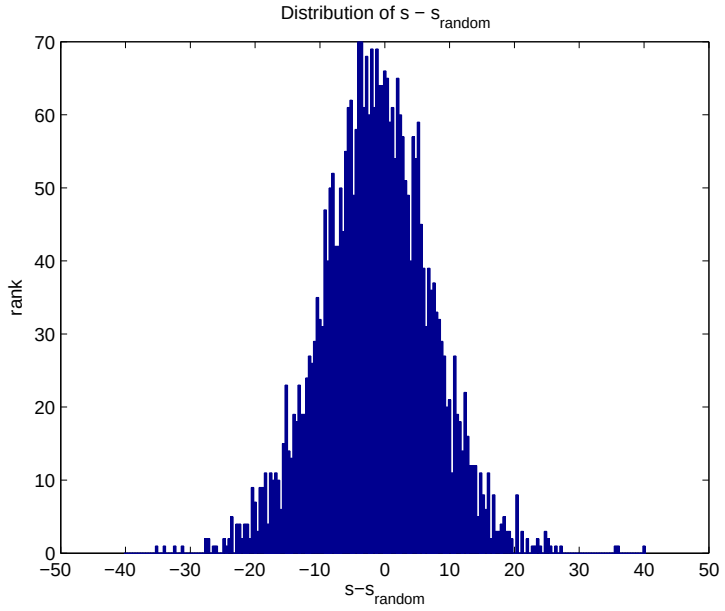

Figure 4.2: Distribution of neighbor correlation relative random reference.

quick transient behavior they fluctuates little around their average value. The fraction of S1T variables increases slightly over time (not monotonic) which indicates that it becomes harder and harder to find ”safe” clause i.e clauses in which a variable can be flipped without creating a new UNSAT clause.

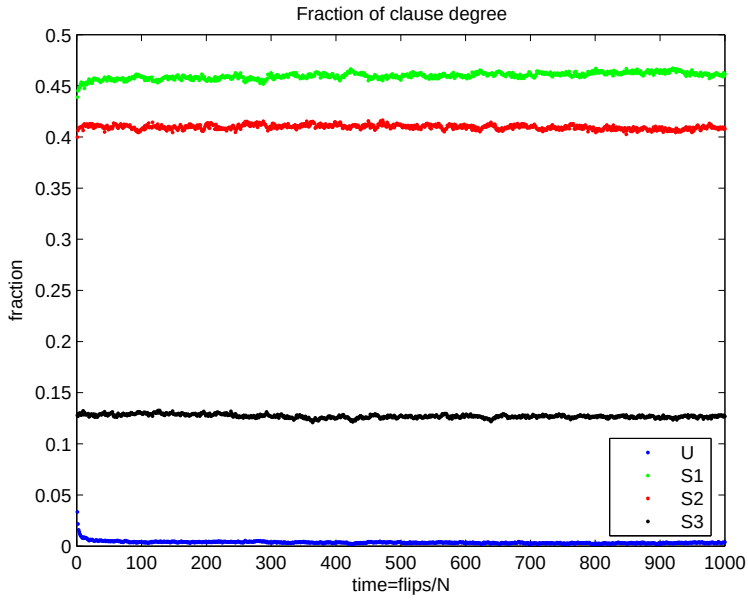

Figure 4.3: Fraction of clauses with different degrees in random 3-SAT.

4.3 Greed vs. waste

The above results indicates that the dynamical behavior of the heuristic is not dependent on details of the current state but rather on averages over some longer timescale. This leads to a suggestion that the dynamics of the SLS heuristics are only dependent on how large, *on average*, the quota between how greedy (decrease in energy is promoted) and wasteful (increase in energy is allowed) the algorithm is. In FMS the probability to do a non optimal flip (up in energy) is weighted with the Boltzmann factor,$e^{1/T}$, for no really apparent reason. If one then assumes that the dynamics is not dependent on energy differences on short timescales one can remove the Boltzmann factor. This leads to a heuristic which makes no difference between a non optimal move close in energy and one further up. That is it resales all local energy barriers to the same level. The heuristic is called *ASAT* (average SAT) and functions like this:

```
s = initial random configuration

while t<t_max
       if F(s) = TRUE then EXIT
       at random pick a unsatisfied clause C
       at random pick a variable x in C

       x' = flip(x)
       s' = s(x -> x')

       if E(s') <= E(s) then flip x else
              flip x with probability p
```

The properties of it are discuessed below.

4.4 Constrained sequences

In a resent work by Seitz et.al [2] it is suggested that the reason for complexity in SAT problems is the onset of large loops. Loops where a flip of an UNSAT variable leads to that one or several other clauses becomes UNSAT.
As a first approach to monitor any kind of periodic looping behavior a list of the number of times a clause has been unsatisfied, denoted *UNSAT list*, was created. At each time step the unsatisfied clauses are marked. After some time comparable to N the list of marks is counted and sorted. The number of marks per clause is plotted in fig 4.4.

Is seems like a few clauses are present more often than others and when iterating through the process this view is confirmed. A couple of the clauses are responsible for the vast part of the presence in the UNSAT list. To validate this fact in a more clear way a rank plot of

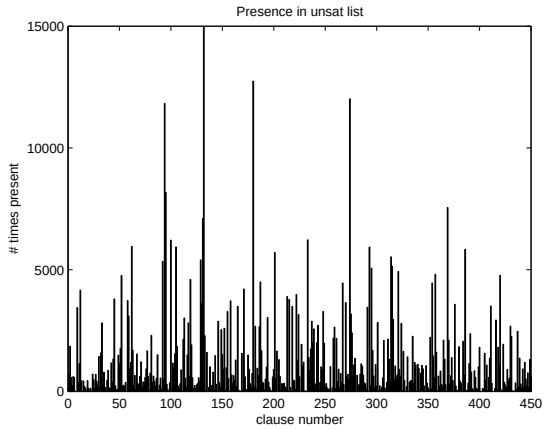

Figure 4.4: Number of times a clause is present in the UNSAT list.

the same data can be found in fig 4.5.

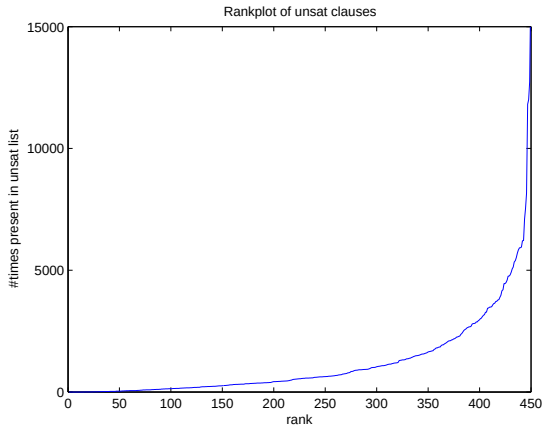

Figure 4.5: Rank plot of presence in the UNSAT list.

The heuristic, when stuck in a metastable state, seems to come across the same few clauses over and over again. This supports the loop idea, that a fraction of the clauses are impossible to satisfy because flipping any of its variables will unsatisfy some other clause. On the other hand, from the plots it is clear that all clauses are unsatisfied at one time or another. This means that even though all variables are flipped sometime during the recording interval the heuristic still is attracted to some "backbone" configuration.

As a last approach to explore the looping theory a FFT (fast Fourier transform) of the return times was done. Return times are the time between when a clause leaves the UNSAT list and when it return the next time. No apparent periods where found in this simulation. Taking this into account it seems like the loops are not at all a sequence of flips but rather an *average pattern* which repeat it self over time. This might explain why ASAT is suc-

cessful in its approach. When the noise parameter is below its critical value (see chap. 5) the probability to enter a sequence which is not attracted to an averages metastable one is to low whereas in optimal configuration it avoids trapping.

4.5 Linear region

The main interest regarding new heuristic methods is to examine the range in α for which the run times are linear in systemsize. This value varies with method and the critical value, α_d, below which the instances are in general solved, is known as the *dynamical phase boundary*. The term dynamical in the title of the thesis refers to this property. The transition is a property of the *dynamics* of the process.

One way to examine the critical α is of course to run the heuristic on a lot of problem instances and plot the run time (e.g. as in sect. 4.1). For random 3-SAT the optimal value of the noise parameter p is 0.22 (the value is determined in chapter 5 and is confirmed numerically).
The optimal value of the noise parameter is however weakly dependent on α. To determine the value of α_d in some detail one therefor is forced to run several instances on several values of α close to the critical value. This procedure is time consuming but reliable.

A lower boundary for α_{lin} seem to be 4.21. Fig 4.6 shows a histogram of run times for the system sizes 10^4, 10^5 and 10^6

It is clear that the run times are self averaging. For the largest systems all the run times are around 10000 flips/N. That is indeed linear.

When the same procedure is done for $\alpha = 4.25$ the picture is somewhat different (Fig. 4.7). Even for relatively small systems the run times are diverging. For $N = 10^4$ (not shown in the picture) no instances are solved below the cutoff. This suggests that the linear region is in the interval. $4.21 < \alpha_{lin} < 4.25$ for ASAT.

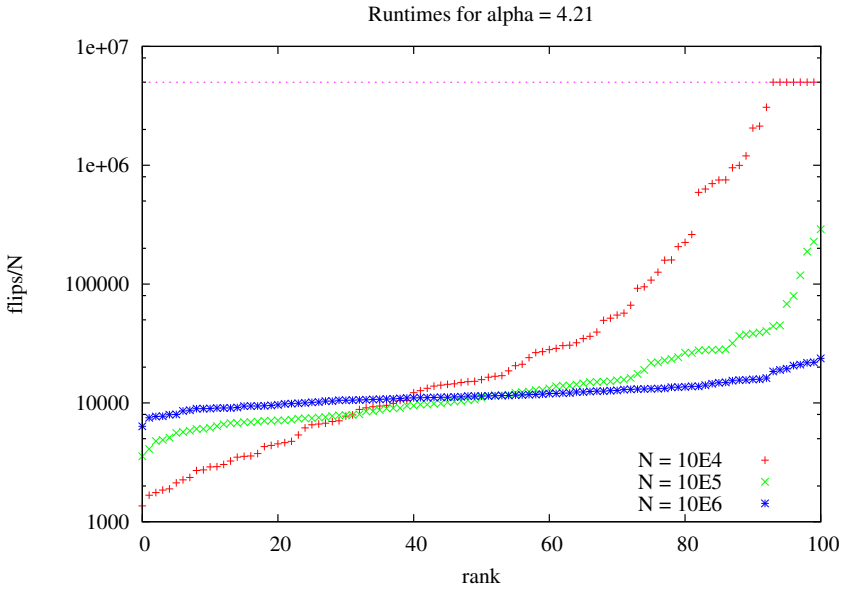

Figure 4.6: Run times for $\alpha = 4.21$. Cutoff is set to $5 * 10^6 N$ flips

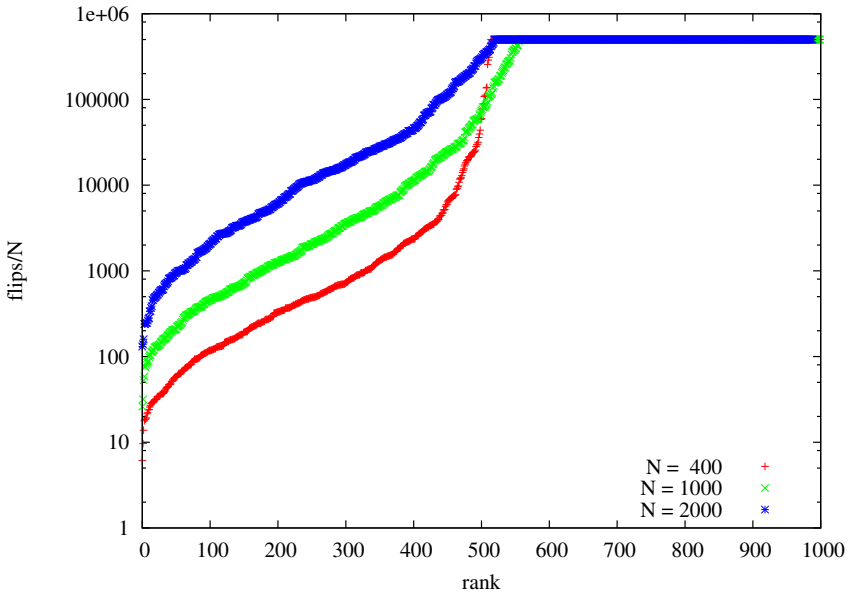

Figure 4.7: Runtimes for $\alpha = 4.25$.

4.6 Time course of solution

Although the linear regime seem to end at $\alpha = 4.21$, ASAT is still able to solve problems even closer to the critical limit. The time course of the solution for $\alpha = 4.22$ is shown below. Here three different behaviors are present. First there is a fast decay of the number

of unsatisfied clauses up to about $t = 2000$ After that a linear regime starts where the number of clauses solved per unit time is approximately constant. It is in this regime that ASAT is able to solve problems for $\alpha < \alpha_{lin}$.
However, for larger α there is an onset of plateaus when only a small part of the clauses are unsatisfied. The process is trapped in some structure for some finite time until it then proceeds to a lower plateau. This behavior continues until the problem i solved. This might be the reason for the exponential run-times. The waiting time on a specific plateau is not deterministic but depends highly on α. This behavior can be seen as an analogy to a phenomenon in complex materials known as *aging*. If the system is left by itself it relaxes on a timescale much longer than the initial equilibrium time. For how high values of α this effect remains is not possible to answer. However it still indicates that there are paths from metastable states to states with even lower energy that does not require crossing an energy barrier. It would therefor in theory be possible to design a heuristic that exploits these 'exits' to decrease the energy.

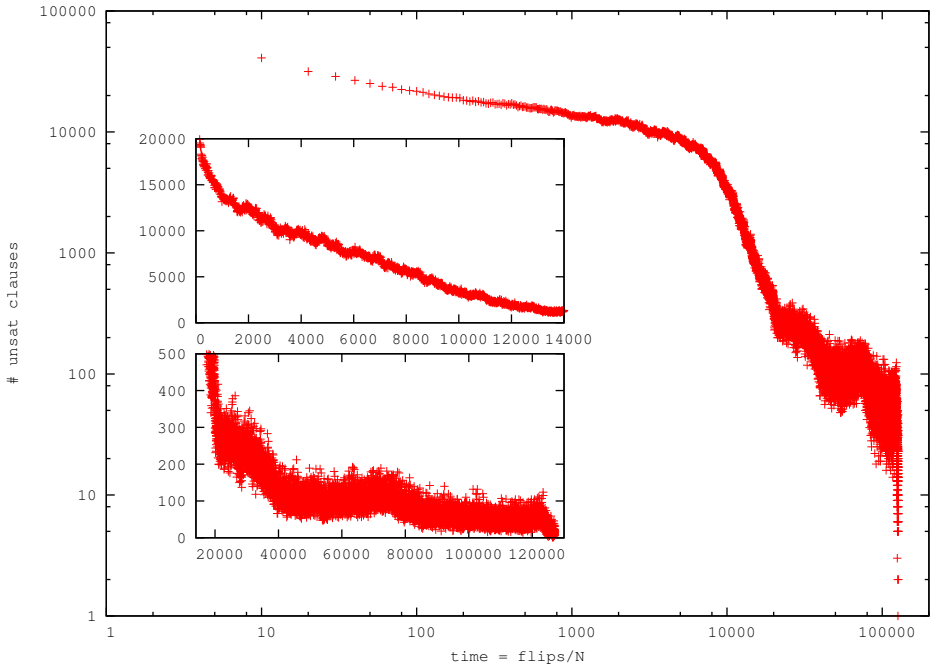

Figure 4.8: Timecouse of solution for $\alpha = 4.22$.

Chapter 5

State space structure

In this chapter some of the relations between states and their dependent external variables such as N and α is examined

5.1 Simulated heating - escape from metastability

As mentioned in chapter 2, according to theory, the state space close to the SAT/UNSAT transition is divided into clusters of solution states. Not only are the clusters divided but the barrier a SLS must cross to move between them have been conjectured to increase with system size [11]. To examine the height of these barriers one can use a method of simulated heating of the system. First we have to define what we mean by distance between two points in a 2^N dimensional space. The natural measure to use in this context is the *Hamming distance* or the self overlap defined as:

$$D_{hamming} = \sum_{i=1}^{N} \delta(s(i) - s'(i)) \tag{5.1}$$

The idea behind this heating procedure is to find a value of the temperature which lets the SLS escape from a metastable state. One assumption made about the dynamics for this to be relevant is that the process is Markovian on timescales $\tau \propto O(N * t_{flip})$. That is the details of *how* the the heuristic ended up in a certain state is not relevant for its future behavior, and fluctuations are small when averaged over τ. Since a state is defined as a configuration which gives a certain energy, two states which are close in a Hamming sense and have essentially the same energy are considered equal. The heating procedure is then:

1. Let the search get trapped in a metastable state. This is easily done by creating an instance close to or above α_c and choosing the initial value of the noise parameter (temperature) low.

2. After a certain amount of time t_{init} do a *zero temperature quench*. That is set the temperature to zero (or at least very low) and let the system equilibrate.

3. After another period τ increase the temperature slightly by Δt followed by a quenching period.

4. Repeat this alternation between temperature increasing and zero temperature.

The initial configuration s is sampled just after t_{init} and the Hamming distance from this point is calculated in each time step. During this procedure the number of unsatisfied clauses, as well as the Hamming distance from the trapped state is monitored. The result of the first run at $N = 10^3$, $\alpha = 4.3$ is shown in fig. 5.1.

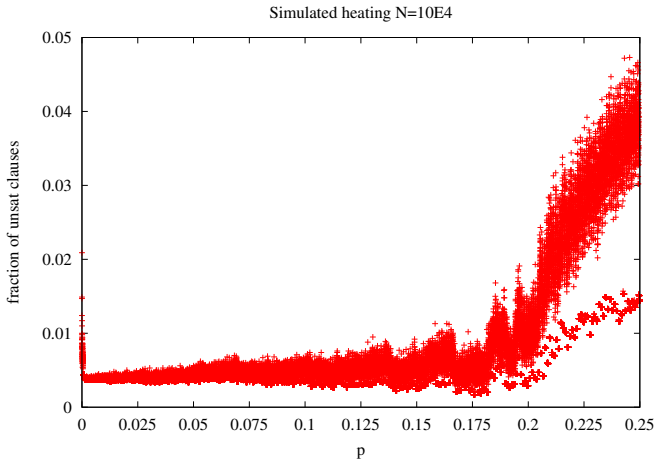

Figure 5.1: Response of UNSAT clauses to increase in temperature.

In the Hamming plot, 5.2, the self overlap between the intial trapped state and the state at time t is shown. The increase in Hamming distance is expected with increasing temperature. What is not expected on the other hand, is that the response in the number of unsatisfied clauses to temperature increase is not a continuous function. Below $p = 0.22$ the system is in the same state (small Hamming distance and same energy). At $p = 0.22$ the system moves out of the metastable state and when it is quenched it returns to the same energy as before, but not at the same Hamming distance. The Hamming distance is now about 3000 which indicates that the correlations between the states are not purely random, but have some parts in common.

Another observation is that below a certain value of the noise parameter p_c the correlations with the initial state is lost and the number of UNSAT variables becomes a continuous function of the temperature. Another observation is that below p_c the zero quenching energy is decreasing with temperature whereas for $p > p_c$ the quenching states reachable have increasing energies. This suggest that above a certain energy (or temperature) some minimas are not reachable by a zero temperature quench, as is familiar from spin glass

models. A closer look at the Hamming distance, plot 5.2, reveals that the system moves through different states within some area from the initial state and then at $p = p_c$ leaves the region. Whether or not these regions are the same as the clusters mentioned in theory is not clear but the simulation clearly indicates some kind of spin glass like structure.
The best value of p would then be just below p_c where the local minimas are accessible and the temperature is high enough to move over small local barriers.

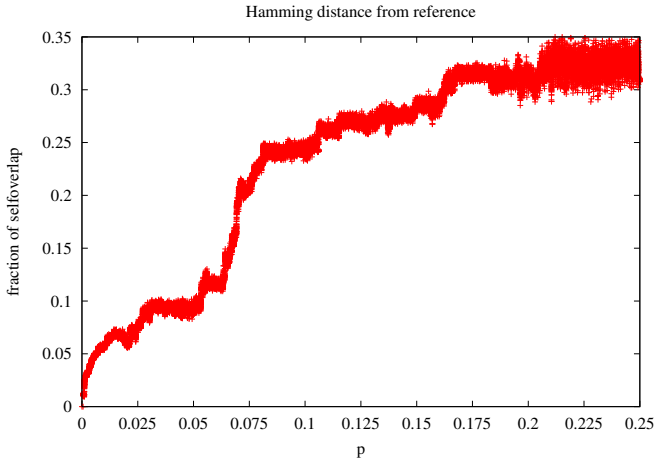

Figure 5.2: Hamming distance from initial metastable state.

5.2 Scaling properties

Important properties of the dynamics as well as statistics of solutions are how they scale with different parameters such as systemsize (N) or clause size (K). Since there are some assumptions that SLS will encounter problems for large N and K scaling is important to examine.

5.2.1 System size scaling

How the system behaves in the thermodynamic limit is of great theoretical as well as practical interest. How large system are one able to solve with a certain method? The scaling of barriers between regions in state space and the scaling of the regions them selfs are some properties which may be effected as the systems grow.
Different predictions have been made and some [11] claims that SLS will face problems due to growing barriers only when the systems becomes very large ($N > 10^6$). However this is not possible to confirm or reject with present computers which have a working memory of about 10^9 bytes. This is a current problem and since there are no rigorous mathematical proofs or strict numerical ones the opinions differ.

In [2] it is suggested that the structure of the state space would be smoother with increasing system size. A view which is reasonable if the reason for complexity is the onset of large loops (see section 4.4). Such effects would decrease with increasing number of variables since the number of neighbors of a variable ($K\alpha$) is independent of N.
In the context of this thesis the only property which one can check with respect to scaling is, apart from the solution times, the critical behavior of the heating simulation carried out in the previous chapter. This is done for a system ten times the size, $N = 10^5$ and the results are shown in fig 5.3.

As one can clearly see, the two plots shows the same general behavior at the same temperature. By this one may conclude one of the following:

- The properties of the metastable states are not dependent on N or at least depend quite weakly on N in the range explored.
- The critical temperature found in the heating simulation is not representative for the noise needed to cross the cluster barriers. Therefore the invariance does not indicate anything regarding the problems SLS might encounter.

5.2.2 Clause size scaling

How properties of the dynamics scale with constraint size is interesting for the same reasons as system size. To examine this the heating simulations is done with K:s in the range [3..10]. The results are show below. The curves display a similar shape as the one for 3-SAT, at some critical temperature the heuristic looses the close connection with the structure and the number of UNSAT clauses increases with energy. The critical temperature is plotted vs. K in fig 5.3.
Another important property is of course how the run-times depend on K. This is however hard to investigate numerically since the number of clauses grows as $K\alpha$ the computer memory will be a limiting factor. Fig. 5.4 shows the run-times for $N = 10^4$ for different values of K.
For these instances there do not seem to be any significant problems occuring with increasing K.

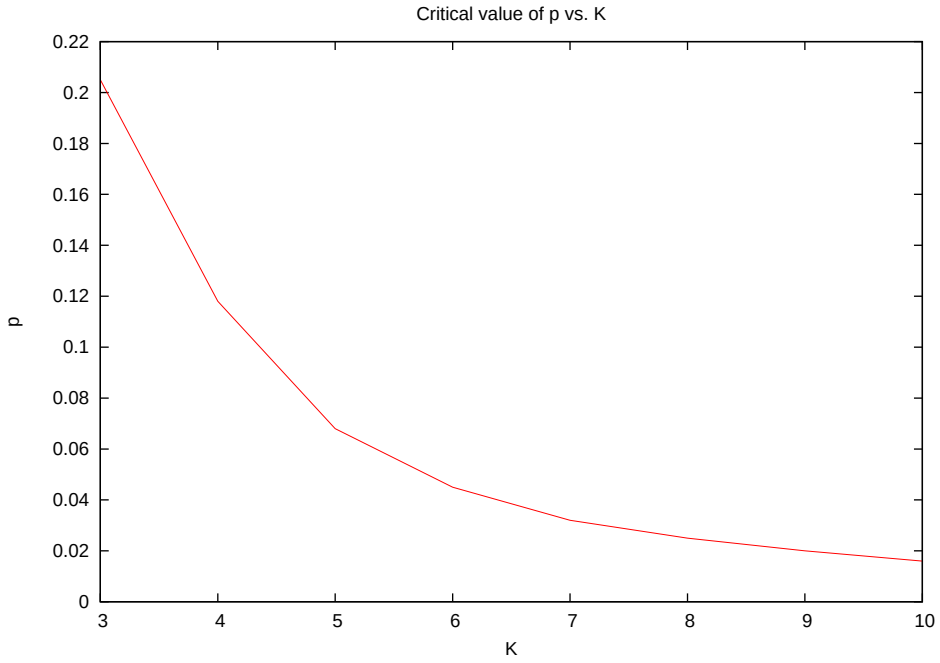

Figure 5.3: Scaling of critical temperature in K.

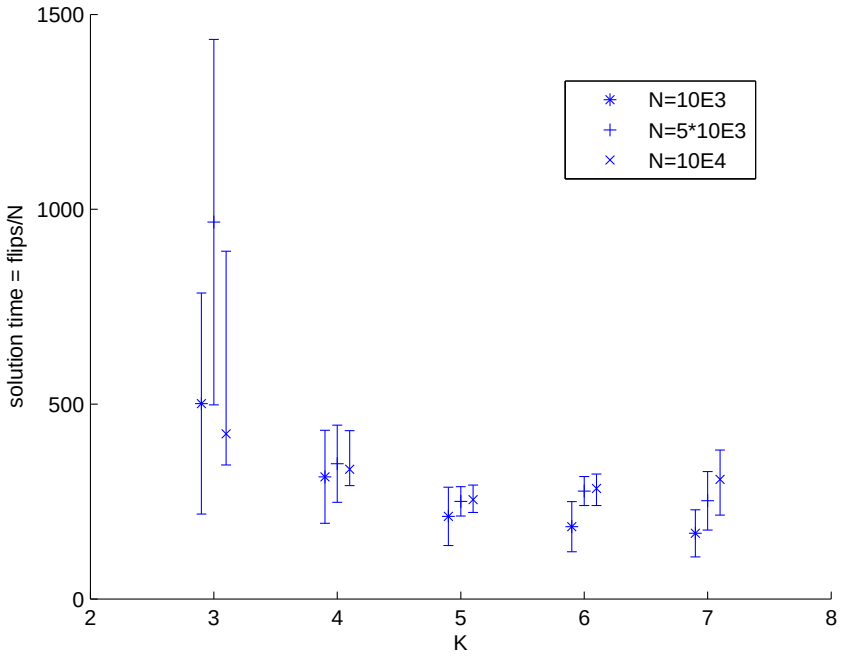

Figure 5.4: Scaling of run times in K.

Chapter 6

Master equation

This chapters contains an analytic approach to model the dynamics of the heuristic solution path of random 3-SAT problems. A rate equation of the probabilities for the system to be in a certain state (master equation) is formulated and analyzed.

6.1 Probability rates

The theoretical approaches mentioned above are all equilibrium methods in the sense that they do not include any transient behavior and are based on statistics of the system at rest. From an algorithmic point of view one would like to be able to model the dynamics that gives rise to the *algorithmic-dependent phase transitions* which may depend heavily on the non-equilibrium dynamics of the system.

In 2003 Barthel et.al approached this problem in a way that is extended here and many of the arguments can be found in [13]. The implementation here is for FMS to make comparison with [13] easier.

First of all let us define the probability

$$p(u, s1, s2, s3) \equiv p(u, \bar{s}) \tag{6.1}$$

to be the probability that a variable in the system is present in u number of unsatisfied clauses, $s1$ number of clauses satisfied by only one variable and so forth.
The initial probability distribution can be approximated by an poissionan distribution:

$$p_0(u, \bar{s}) = e^{-K\alpha} \frac{(K\alpha_u)^u (K\alpha_{s_1})^{s_1} (K\alpha_{s_2})^{s_2} (K\alpha_{s_3})^{s_3}}{u! s_1! s_2! s_3!} \tag{6.2}$$

The specific rules of the heuristic is modeled using step function:

$$q_{flip}(x, y) = \frac{1}{2}\eta(x - y)\Theta(x - y) + \Theta(y - x)\frac{1}{2} \tag{6.3}$$

$$\Theta(x-y) = \begin{cases} 1 & x = y \\ 0 & x < y \\ 2 & x > y \end{cases} \tag{6.4}$$

If a variable belongs to a s_1 clause it is by probability $(\frac{1}{3})$ the sole satisfying variable. This fact is taken care of by another function (assumed to be binomial distributed):

$$q(a,b) = (\frac{1}{2})^a (\frac{2}{3})^b \binom{a+b}{a} \tag{6.5}$$

Another convention that is used in the equation is the average of a variable:

$$< u >= \sum_{u,s_1,s_2,s_3} up(u,s_1,s_2,s_3) \tag{6.6}$$

6.1.1 Rate equations

The number of variables that belong to unsatisfied clauses can be altered if that clause is picked. This is done with probability $p_{flip} = \frac{up(u,\bar{s})}{<u>}$. There are also a possibility for any number out of the current s_1 variables to, by a flip, make their clause satisfied. This is considered by summing over all possible s_1 states. On the other hand variables can be flipped to turn clauses unsatisfied which is the gain term below.

$$\begin{aligned} \frac{dp(u,\bar{s})}{dt} &= -p_{flip} \sum_{\tilde{u}=0}^{s_1} q(\tilde{u}, s_1 - \tilde{u}) q_f(u,\tilde{u}) \\ &+ \sum_{\tilde{u}=0}^{s_1+u} p(\tilde{u}, s_1 + u - \tilde{u}, s_2, s_3) \frac{\tilde{u}}{< u >} q(u, s - \tilde{u}) q_f(u,\tilde{u}) + \end{aligned} \tag{6.7}$$

The next step is to consider the other variables that belong to the same clauses as the flipped ones. These are the so called *neighbor* and there are 2 neighbors in each of the u clauses. So the change in state of these variables is either to increase the number of satisfied clauses the variable belongs to or decreased the number of unsatisfied clauses (gain and lose terms below).

$$\begin{aligned} &+ \sum_{u',s_1',s_2',s_3'} \Big\{ \frac{u' P(u',\bar{s'}}{< u >} \sum_{\tilde{u}=0}^{s_1^a} q(\tilde{u}, s_1^a - \tilde{u}) q_f(u,\tilde{u}) \\ &\quad * 2u' \Big\} \Big\{ \frac{(u+1)p(u+1.s_1-1, s_2, s_3)}{< u >} - \frac{up(u,\bar{s})}{< u >} \Big\} + \end{aligned} \tag{6.8}$$

Lets now consider the clauses satisfied by 1 variable, the s_1's. By the same arguments as for the unsatisfied clauses. The number of such can increase if an u variable is flipped and decreased if an s_2 variable is.

$$
\begin{aligned}
&+\sum_{u',s^{\bar{a}}}\Big\{\frac{u'P(u',s^{\bar{a}})}{<u>}\sum_{\tilde{u}=0}^{s_1^a}q(\tilde{u},s_1^a-\tilde{u})q_f(u,\tilde{u})\Big\}\\
&\quad\Big\{2\tilde{u}\Big\{\frac{(s_1+1)p(u-1.s_1+1,s_2,s_3)}{<s_1>}-\frac{s_1p(u,\bar{s})}{<s_1>}\Big\}\\
&\quad 2(s'^a-\tilde{u})\Big\{\frac{(s_1+1)p(u.s_1+1,s_2-1,s_3)}{<s_1>}-\frac{s_1p(u,\bar{s})}{<s_1>}\Big\}+
\end{aligned}
\tag{6.9}
$$

There are also neighbors in the s_2 type clauses which are effected by a the flip. Now one must consider the number of clauses in which a variable is the sole unsatisfying variable, denoted $\tilde{\tilde{u}}$

$$
\begin{aligned}
&+\sum_{u',s^{\bar{a}}}\frac{u'P(u',s^{\bar{a}})}{<u>}\sum_{\tilde{u}=0}^{s_1^a}q(\tilde{u},s_1^a-\tilde{u})q_f(u,\tilde{u})\\
&\quad *\sum_{\tilde{\tilde{u}}=0}^{s_2^a}q(\tilde{\tilde{u}},s_2^a-\tilde{\tilde{u}})\Big\{2\tilde{\tilde{u}}\Big\{\frac{(s_2+1)p(u,s_1,s_2+1,s_3-1)}{<s_2>}-\frac{s_2p(u,\bar{s})}{<s_2>}\Big\}\\
&\quad +2(s_2^a-\tilde{\tilde{u}})\Big\{\frac{(s_2+1)p(u,s_1-1,s_2+1,s_3)}{<s_2>}-\frac{s_2p(u,\bar{s})}{<s_2>}\Big\}\Big\}+
\end{aligned}
\tag{6.10}
$$

The last part of the neighbor interactions is to consider the number of flipped variables in the s_3 type clauses.

$$
\begin{aligned}
&+\sum_{u',s^{\bar{a}}}\frac{u'P(u',s^{\bar{a}})}{<u>}\sum_{\tilde{u}=0}^{s_1^a}q(\tilde{u},s_1^a-\tilde{u})q_f(\tilde{u},u)\\
&\quad *2s_3^a\Big\{\frac{(s_3+1)p(u,s_1,s_2-1,s_3+1)}{<s_3>}-\frac{s_3p(u,\bar{s})}{<s_3>}\Big\}
\end{aligned}
\tag{6.11}
$$

The sum of all the terms is implemented in MATLAB. It seems that number of variables needed to represent the distribution is about 30 for each variable. That is the operations are done on matrices with the size of 30^4 variables. This value is dependent on α and 30 is for $\alpha = 3$. Figure ... shows the time course of solution for $\alpha = 3$. Unfortunately the results of the simulations is not in agreement with [13]. The problems are solved for to high values of α. To rule out any bugs in a code like this is a hard task especially when all easy checks like $\sum p(u,\bar{s}) = 1$ etc. are fulfilled. There is however no doubt that some treatment along these lines will be successful.

Chapter 7

Discussion and outlook

In this thesis a new heuristic named ASAT is introduced which seem to be simpler and faster than the existing ones. This gives hope for a more analytic analysis which will shed light on non-equilibrium processes encountered in combinatorial optimization. Another application of ASAT is the ability to explore the state space seen be the heuristic. It appears as the local structure of the state space is only weakly dependent on the size of the system. The critical value of the order parameter can be tuned to be high enough to escape these local minimas but low enough to explore the lower parts of them.
Considering the simplicity of ASAT further development of heuristic will probably have to focus on average properties of states rather than the details of current state.
Although the system sizes investigated in this theses are large one can never rule out that one can encounter problems for even larger systems. In practical applications, systems larger then 10^6 variables are uncommon. This will probably demand a theoretical analysis to determine such upper boundary. Apparently the clustering transition is not the upper limit for the efficiency of heuristic methods. Even though the local barriers do not grow extensively with N the barriers between different clusters may. However this is not a problem in optimization problems, as long as one is able to find at least one optimal solution. How well ASAT and other similar heuristics are doing on real problems (where the constraints are not random) is also left to investigate.

From a pure theoretical point of view one would like to have some more rigorous way to analyze these process. To understand the interplay between statistics and dynamics in theses systems would be a great step towards a more profound understanding of non-equilibrium processes in general. There are many questions left unanswered like Why is focused search so efficient? Can a Markovian process be successful on theses systems or do the strategies demand information from several subsequent steps? Are there mappings from behavior in the dynamics to structure in the state space of complex problems? Heuristic methods can indeed be of some usage in the search for answers.

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