On the behaviour of random $K$-SAT on trees

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Abstract. We consider the $K$-satisfiability problem on a regular $d$-ary rooted tree. For this model, we demonstrate how we can calculate in closed form the moments of the total number of solutions as a function of $d$ and $K$, where the average is over all realizations for a fixed assignment of the surface variables. We find that different moments pick out different ‘critical’ values of $d$, below which they diverge as the total number of variables on the tree $\rightarrow \infty$ and above which they decay. We show that $K$-SAT on the random graph also behaves similarly. We also calculate exactly the fraction of instances that have solutions for all $K$. On the tree, this quantity decays to 0 (as the number of variables increases) for any $d > 1$. However, the recursion relations for this quantity have a non-trivial fixed point solution which indicates the existence of a different transition in the interior of an infinite rooted tree.

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1. Introduction

Constraint satisfaction problems (CSPs) are problems in which a set of variables, which can take values in a specified domain, has to satisfy a number of constraints. Each constraint usually restricts the values that a subset of the variables can take. The problem then is to find an assignment of the variables that satisfies all the constraints. The $K$-satisfiability problem ($K$-SAT) is an important example of a CSP. In this problem, the variables are considered Boolean, taking values true or false, and each constraint is in the form of a clause, which restricts the values of $K$ variables at a time, disallowing 1 out of the $2^K$ possible values that these $K$ variables can take together.

Satisfiability has been a fundamental problem for almost forty years in computer science. It is known that as soon as there are clauses which restrict the values of $K \geq 3$ variables, this problem is nondeterministic polynomial time complete (NP-complete) [1], i.e. potential solutions can be verified easily for correctness, but finding a solution can take exponential time in the worst case. In addition, being NP-complete, should a polynomial-time algorithm be found for solving SAT, it is also possible to adapt it to solve in polynomial time all problems in NP.

The version of the $K$-SAT that we are interested in, in this paper, is the random $K$-SAT, which has been very well investigated in the past few years. In the random $K$-SAT one looks at the ensemble of randomly generated logical expressions, where each logical expression or formula is an AND of $M$ clauses. Each clause consists of an OR of $K$ Boolean literals (a literal being one of the $N$ variables or its negation), chosen randomly.
randomly from a set of $N$ Boolean variables. As the ratio $\alpha = M/N$ increases it becomes harder to find satisfiable assignments for all the $N$ variables that can satisfy the logical expression of $M$ clauses. One of the questions of interest is hence if there exist $\alpha_c$, beyond which in the limit of $M \to \infty$ and $N \to \infty$, no satisfying assignments exist.

Numerical experiments have shown in the past that if one studies the probability that a randomly chosen formula having $M = \alpha N$ clauses is satisfiable, the probability approaches 1 for $\alpha < \alpha_c(K)$ and vanishes for $\alpha > \alpha_c(K)$ when $N \to \infty$ [2, 3]. The existence of a sharp transition (the solvability transition) is intrinsic to the problem and not an artefact of any particular algorithm (in [4] the existence of a possibly $N$-dependent transition is proved for any $K$), but its location has not been determined rigorously with the exception of $K = 2$ [5]. There are, however, several rigorous bounds on $\alpha_c(K)$, both upper and lower (see [6] for a review of these). In addition, powerful methods from statistical physics, taking advantage of the connection of this problem to the theory of mean field spin glasses, have been used to conjecture values for the threshold that seem to be very accurate numerically [7, 8].

The above problems are all originally defined on random graphs, where the presence of large loops makes the problem hard to solve exactly. Hence solving the problem on trees or locally tree-like graphs has played an important role in elucidating the nature of the solvability transition as well as other phase transitions present in the problem. In fact the methods from statistical physics assume the absence of correlations between some random variables, which is equivalent to solving the $K$-SAT problem on a locally tree-like graph. In addition, it has also been shown that certain problems on a tree, in particular the tree-reconstruction problem [9], become equivalent to the spin glass problem on a random graph.

In this paper we study the $K$-SAT problem on a regular $d$-ary rooted tree in which every vertex (except the leaves) has exactly $d$ descendants. The values that the surface nodes (or leaves) take on the tree, are fixed. For a given assignment of the surface nodes, and a given realization of clauses on the tree, one can ask how many assignments of the variables on the tree are solutions. For such a tree graph, we can exactly calculate the moments of this quantity averaged over all realizations. The behaviour of the moments is similar to that on the random graph, and we find that there is a different ‘critical’ point associated with each moment as in the random energy model considered by Derrida [10]. We also calculate exactly the fraction of realizations that have solutions, for a tree of any size. This property too shows a similarity to the behaviour of the model on a random graph, since there is a value of $d$ above which the fraction of realizations that have solutions $\to 0$ as $N \to \infty$. We also look at this quantity in the interior of an infinite tree, and show that a different transition takes place in this limit.

The plan of the paper is as follows: in section 2 we introduce the model. In sections 3-5 we calculate the moments of the number of assignments that are solutions averaged over all realizations for a randomly fixed boundary, for 2-SAT, 3-SAT and arbitrary $K$ respectively. In section 6, we calculate the probability that a given realization has at least one solution (or equivalently the fraction of realizations that have solutions), as a function of the depth of the tree. In section 7, we carry out the fixed point analysis relevant for the interior of an infinite tree. We end with a summary and discussion in section 8.
2. The model

We define the $K$-SAT problem on a tree as follows. Consider a regular $d$-ary tree $T$ in which every vertex has exactly $d$ descendants. The root of the tree $x_0$ has degree $d$ and its $d$ edges are connected to function nodes $\{c_1, c_2, \ldots, c_d\}$. Each function node has degree $K$, and each of its $K-1$ descendants $\{x_i = x_1, x_2, \ldots, x_{k-1}\}$ is the root of an independent tree (see figure 1). Hence the root has a degree $d$ while all the other vertices on the tree (except the leaves which have a degree =1) have a degree $d + 1$. Each function node is associated independently with a clause $\phi(x_0, x_1, \ldots, x_{k-1})$, where the vertices $x_0, x_1, \ldots$ are the neighbouring vertices of the function node, joined to the function node by a dashed or solid edge indicating whether the corresponding vertex is negated or not in the clause. We consider only the case where the vertices can take one of two values 0 or 1 and the case when every function node is given by $\phi = \ell_0 \lor \ell_1 \lor \cdots \lor \ell_{k-1}$. Here $\ell_i$ is one of the two literals $x_i$ or $\overline{x_i}$, depending on whether $x_i$ is joined to the function node by a dashed or a solid line (figure 1).

An assignment $\sigma$ of all the variables on the tree (barring the surface variables which take fixed values, see below) is a solution iff $\phi = 1$ for all the clauses on the tree. One configuration of dashed and solid lines on the tree defines a realization $R$.

For a random $K$-SAT problem, i.e. a $K$-SAT problem on a random graph, the variable $\alpha = M/N$ where $M$ is the total number of clauses and $N$ is the total number of variables (vertices), is a meaningful quantity. As a function of this one can ask, for example, how the moments of the total number of solutions (averaged over all realizations) scale with $N$.

To ask the same question meaningfully here on a tree, it is usual to fix the values of the variables on the surface of the tree. If we consider the surface variables to have depth 0, then we can denote this condition by $\sigma(0) = L$, where $\sigma(0)$ is the assignment of the variables at the 0th depth and $L$ signifies a particular assignment for the variables at this depth. Variables removed from the surface by one function node (or one level) are at depth 1 and so on. The tree is said to have a depth $n$ if the root is $n$ levels away from the surface.

If the surface variables are fixed, then it is easy to check that $M(n) = dN(n)$, where $M(n)$ and $N(n)$ are respectively, the total number of clauses for a tree of depth $n$ and the
total number of vertices ($d = 1$ if the surface variables are left free). So $\alpha$ is the equivalent of $d$ on a tree with fixed boundary conditions.

Let us denote the total number of solutions (a sum over all $\sigma$ which are solutions) for a particular realization of a tree of depth $n$ and a specific boundary condition $L$ as $Z_R(L, n)$. This is a stochastic variable which varies from realization to realization as well as from one boundary condition to another. The first moment of this quantity, averaged over all realizations (for a fixed boundary condition), is trivially computed and is equal to $((2^K - 1/2^K)d)^2 N(n)$ (we derive this later in section 3). In this case, if $(2^K - 1/2^K)d^2 > 1$, then the number of solutions grows as the tree gets bigger and if $(2^K - 1/2^K)d^2 < 1$, then the number of solutions decreases as the number of variables grows. The critical point of the first moment is therefore at $(2^K - 1/2^K)d^2 = 1$. This gives $d_c = -\log(2)/\log(1 - 2^{-K})$. Note that, from simple considerations, it is easy to see that even the random $K$-SAT has the same expression for the first moment as on the tree, with $d$ replaced by $\alpha$. This expression for the first moment gives an annealed approximation for $\alpha_c(K)$.

We are henceforth interested in also estimating the higher moments for $Z_R(L, n)$. Before writing down the recursions for this quantity on the tree, however, we introduce a little more notation. By $C^s(x_i)$ we denote all the clauses which are neighbours of variable $x_i$ and are satisfied by it. Similarly, by $C^n(x_i)$ we denote all the clauses which are neighbours of variable $x_i$ but are not satisfied by it. Let $F_R(L, n)$ and $G_R(L, n)$ denote the number of solutions for a tree of depth $n$ (for a given realization and boundary condition $L$) in which the root takes the value 0 and 1 respectively.

3. Recursion relations on the tree for 2-SAT

We can write the exact recursion equations on the tree for the stochastic variable $Z_R(L, n)$. We first look at the form of these recursions for 2-SAT. For ease of notation we henceforth omit the $L$ in the argument. A rooted tree of depth $n$ is generated by taking a root of degree $d$, then picking, for all edges connecting the root to the function node, independently of the type of edge (dashed or solid) and finally attaching trees of depth $n - 1$ to the other end of the function node (again via edges that are independently chosen to be dashed or solid), see figure 2.

Let $d_1$ be the cardinality of the set $C^n(x_0)$, when vertex $x_0$ takes value 0. Then the vertices along the other edge of these clauses can only take on the specific value satisfying the clause, for any realization of the edge connecting them to the clause. For those clauses satisfied by $x_0$ ($d - d_1$ of them; $d - d_1$ is just the cardinality of the set $C^s(x_0)$), the vertex at the other edge of the clause is free to take any value. So the number of solutions for the tree of depth $n$, with root node taking value $x_0 = 0$, for this specific realization (and boundary condition), is the product of the number of solutions of $d$ subtrees of depth $n - 1$.

The recursion relation for $F_R$ is hence:

$$F_R(n) = \prod_{i=1}^{d-d_1} Z_{R_i}(n-1) \prod_{i=d-d_1+1}^{d} \left( (F_{R_i}(n-1)\eta_i + G_{R_i}(n-1)(1-\eta_i)) \right) \tag{1}$$

where $R_i$ denotes the realization of each of the subtrees rooted in the descendants of $x_0$ and $\eta_i$ is a stochastic variable which is equally likely to take the value 0 or 1, depending
Figure 2. Schematic diagram of the tree for 2-SAT. Variable $x_0$—the root of a tree of depth $n$—is connected through clauses $c_1$, $c_2$ and $c_3$ to variables $x_1$, $x_2$ and $x_3$ respectively, each of which is in turn the root of a tree of depth $n - 1$.

on whether the edge joining the variable at depth $n - 1$ to its clause is dashed or solid. Similarly,

$$G_R(n) = \prod_{i=d-d_1+1}^{d} Z_{R_i}(n-1) \prod_{i=1}^{d-d_1} (F_{R_i}(n-1)\eta_i + G_{R_i}(n-1)(1-\eta_i)) \quad (2)$$

and

$$Z_R(n) = G_R(n) + F_R(n). \quad (3)$$

We can define, $\beta_R(n) \equiv F_R(n)/Z_R(n)$ as the fraction of solutions in which the root $x_0$ takes the value 0 for a given realization $R$ and a fixed but arbitrary boundary condition $L$. Note then that if, for a given $R$, we selectively sum over those boundary conditions which result in a certain $\beta_R(n)$, this gives the recursion for the residual distribution at the root derived earlier in the context of tree reconstruction in [9,11].

Our interest here, however, is to calculate the moments of $Z_R(n)$ from the above recursion relations by averaging over all realizations, for an arbitrary boundary condition $L$. Hence by $\langle F_R(n) \rangle$, we will denote an average over all realizations $R$ for a tree of depth $n$. It is easy to see that such an average is achieved at the root, by averaging over all possible $d_1$s for a given $d$, where the probability that there are $d_1$ clauses unsatisfied by the root is given by the binomial distribution $P(d_1) = 1/2^d \binom{d}{d_1}$. Also note that since different branches of the tree are independent of each other, we have,

$$\langle F_{R_i}(n)F_{R_j}(n) \rangle = \langle F_{R_i}(n) \rangle \langle F_{R_j}(n) \rangle = \langle F_{R}(n) \rangle^2 \quad (4)$$

where $i$ and $j$ are variables along different branches. In addition,

$$\langle F_{R_i}(n) \rangle = \langle G_{R_i}(n) \rangle \quad (5)$$

by symmetry. In fact this is true for any moment of $F$ (or $G$). It is also easy to see that

$$\langle \eta_i \rangle = 0.5 \quad (6)$$

$$\langle \eta_i(1-\eta_i) \rangle = 0 \quad (7)$$

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and

\[ \langle \eta_i \eta_j \rangle = \langle \eta_i \rangle \langle \eta_j \rangle = 0.25. \] (8)

Using the above equations, we can now solve equation (1) to obtain the different moments.

### 3.1. First moment or average number of solutions

The average number of solutions as discussed earlier, can be obtained by just looking at the probability of satisfying individual clauses. In this section we average equation (1) and make use of equation (5) to obtain (after removing subscripts for ease of notation):

\[ \langle Z(n) \rangle = 2 \langle F(n) \rangle \] (9)

and

\[ \langle F(n) \rangle = \frac{1}{2^d} (\langle Z(n-1) \rangle + \langle F(n-1) \rangle)^d \] (10)

\[ \langle F(n) \rangle = \left( \frac{3}{4} \right)^d \langle Z(n-1) \rangle^d \] (11)

which implies

\[ \langle Z(n) \rangle = 2 \left( \frac{3}{4} \right)^d \langle Z(n-1) \rangle^d. \] (12)

This is a simple recursion relation which we can solve easily for any boundary condition. The recursion relation at the boundary is

\[ \langle Z(1) \rangle = 2 \left( \frac{3}{4} \right)^d \] (13)

and

\[ \langle F(1) \rangle = \left( \frac{3}{4} \right)^d. \] (14)

Equation (13) follows from equation (12) by noting that \( Z(0) = 1 \). Using the boundary condition equation (13), we can solve the recursion relation equation (12) to get the same result for the average number of solutions as mentioned in section 2.

### 3.2. Second moment

To get the second moment, note

\[ \langle Z^2(n) \rangle = 2 \langle F^2(n) \rangle + 2 \langle F(n) G(n) \rangle. \] (15)

From the recursion equation (1) for the stochastic variable \( F_R(n) \), we have

\[ F^2_R(n) = \prod_{i=1}^{d-d_1} Z^2_R(n-1) \prod_{i=d-d_1+1}^d (F_R(n-1) \eta_i + G_R(n-1)(1-\eta_i))^2. \] (16)
This gives (again getting rid of subscripts)

\[
\langle F^2(n) \rangle = \frac{1}{2^d} \left( \langle Z^2(n-1) \rangle + \langle F^2(n-1) \rangle \right)^d
\]

(17)

\[
= \frac{1}{2^d} \left( \langle 2F^2(n-1) + 2F(n-1)G(n-1) \rangle + \langle F^2(n-1) \rangle \right)^d
\]

(18)

\[
= \left( \frac{3}{2} \langle F^2(n-1) \rangle + \langle F(n-1)G(n-1) \rangle \right)^d.
\]

(19)

Similarly the equation for \( \langle F(n)G(n) \rangle \) is

\[
\langle F(n)G(n) \rangle = \left( \langle F^2(n-1) \rangle + \langle F(n-1)G(n-1) \rangle \right)^d.
\]

(20)

These two coupled equations need to be solved to get the second moment. The boundary conditions are,

\[
\langle F^2(1) \rangle = \left( \frac{3}{2} \right)^d
\]

(21)

which we get by noting that \( \langle F^2(0) \rangle = 1/2 \) and \( \langle F(0)G(0) \rangle = 0 \). Similarly,

\[
\langle F(1)G(1) \rangle = \left( \frac{1}{2} \right)^d.
\]

(22)

To solve the coupled recursion equations, let us define the ratio

\[
r_n \equiv \frac{\langle F_R(n)G_R(n) \rangle}{\langle F^2_R(n) \rangle}.
\]

(23)

Then we have the following equation for \( r_n \).

\[
r_n = \frac{[1 + r_{n-1}]^d}{[3/2 + r_{n-1}]^d}
\]

(24)

with boundary condition \( r_1 = \left( \frac{2}{3} \right)^d \).

For large \( n \), \( r_n \) reaches a fixed point and in that limit we can solve for the fixed point of this equation to get \( r^* = 0.78(d = 1), 0.576(d = 2), 0.4(d = 3) \). If we now approximate the equation for

\[
\langle F^2(n) \rangle \sim \langle F^2(n-1) \rangle^d(3/2 + r^*(d))^d.
\]

(25)

We can solve this to get (for \( d > 1 \))

\[
\langle F^2(n) \rangle \sim \left[ \frac{1}{2}(3/2 + r^*(d))^{1/d-1} \right]^d
\]

(26)

If the term in the brackets is \(<1\), the second moment decreases with system size. If it is \(>1\), then the second moment increases with system size. The ‘critical’ value lies between \( d \sim 3.1 \) and 3.2. To get the value of this threshold more precisely, we need to solve the equation

\[
\langle F^2(n) \rangle \sim \langle F^2(n-1) \rangle^d(3/2 + r_{n-1}(d))^d
\]

(27)

exactly. Solving it numerically we get the critical value of \( d \) to lie between 3.06 and 3.07.

We can follow this procedure for any moment, though the number of coupled recursions that have to be solved simultaneously increases with the order of the moment.
4. Recursion relations for $K = 3$

The recursion relations for higher $K$, though slightly more complicated, follow the same logic as for $K = 2$. We carry out the computation for $K = 3$ here. Now the recursion relation for $F_R(n)$ is

$$F_R(n) = \prod_{i=1}^{d-d_1} Z_{R_{i1}} Z_{R_{i2}} \prod_{i=d-d_1+1}^{d} [Z_{R_{i1}} Z_{R_{i2}} - (F_{R_{i1}} \eta_{i1} + G_{R_{i1}} (1 - \eta_{i1}))]$$

$$\times (F_{R_{i2}} \eta_{i2} + G_{R_{i2}} (1 - \eta_{i2}))$$

where we have removed the dependence on $n - 1$ in the LHS for ease of presentation. We can also write a similar equation for $G$. The $\eta$s are the same as appear earlier. The $i1$ and $i2$s signify the two variables at the end of the same clause, (see figure 1). Since they belong to two different branches, their averages still decouple. The second term is the counterpart of the term appearing in 2-SAT along the branches where the root was not satisfying the clause (or link in 2-SAT). In the case of 3-SAT, if the root does not satisfy one of it clauses, the other two variables are collectively constrained to not take 1 out of the 4 total assignments they could have had. Which specific assignment is forbidden depends on the realization.

4.1. First moment or average number of solutions

Again removing subscripts,

$$\langle F(n) \rangle = \frac{1}{2^d} (\langle Z(n-1) \rangle^2 + \langle Z(n-1) \rangle^2 - \langle F(n-1) \rangle^2)^d$$

$$\langle F(n) \rangle = \frac{1}{2^d} (2\langle Z(n-1) \rangle^2 - \langle F(n-1) \rangle^2)^d$$

$$= (\frac{7}{8})^d \langle \langle Z(n-1) \rangle \rangle^{2d}$$

implying

$$\langle Z(n) \rangle = 2(\frac{7}{8})^d \langle \langle Z(n-1) \rangle \rangle^{2d}.$$  

As before, we need to solve the recursion relations keeping the boundary conditions in mind. The recursion relation at the boundary is

$$\langle Z(1) \rangle = 2(\frac{7}{8})^d$$

and

$$\langle F(1) \rangle = (\frac{7}{8})^d.$$  

We can now solve equation (32) to get the result for the annealed average, already mentioned in section 2.
4.2. Second moment

Squaring equation (28) and taking averages, we get

\[
\langle F^2(n) \rangle = \left\langle \prod_{i=1}^{d-d_1} Z_{i1}^2(n-1) Z_{i2}^2(n-1) \prod_{i=d-d_1+1}^d (Z_{i1} Z_{i2} - (F(n-1)\eta_1 + G(n-1)(1-\eta_1))) \right\rangle \times (F(n-1)\eta_2 + G(n-1)(1-\eta_2))^2.
\] (35)

Simplifying, we get

\[
\langle F^2(n) \rangle = \frac{1}{2d}(\langle Z^2(n-1) \rangle^2 + \langle Z^2(n-1) \rangle^2 - 2\langle F(n-1)Z(n-1) \rangle^2)^d
\]

\[
= \frac{1}{2d}(7\langle F^2(n-1) \rangle^2 + 6\langle F(n-1)G(n-1) \rangle^2 + 12\langle F(n-1)G(n-1) \rangle\langle F^2(n-1) \rangle)^d.
\] (37)

Similarly the equation for \(\langle F(n)G(n) \rangle\) is

\[
\langle F(n)G(n) \rangle = (3\langle F^2(n-1) \rangle^2 + 3\langle F(n-1)G(n-1) \rangle^2 + 6\langle F(n-1)G(n-1) \rangle\langle F^2(n-1) \rangle)^d.
\] (38)

Again defining the ratio of \(\langle F(n)G(n) \rangle\) to \(\langle F^2(n) \rangle\) as \(r_n\), we get

\[
r_{n+1} = \left[\frac{3 + 3r_n^2 + 6r_n}{7/2 + 3r_n^2 + 6r_n}\right]^d
\] (39)

with \(r_1 = (6/7)^d\).

Going through the same procedure as before, we find that the second moment diverges for \(d < 7.16\). In comparison, the first moment diverges for \(d < 5.19\).

5. Recursion relations for arbitrary \(K\)

Similarly, we can easily write the recursions for \(F_K(n)\) for any \(K\). Skipping details, the equation for the \(r_n\)s and for \(\langle F^2(n) \rangle\) for arbitrary \(K\) are

\[
r_{n+1} = \left[\frac{(2K-1) - 1 + g(r_n)}{(2K-1) - 0.5 + g(r_n)}\right]^d
\] (40)

where

\[
g(r_n) = (2^{K-1} - 1) \sum_{i=0}^{K-2} \binom{K-1}{i} r_n^{K-1-i}
\] (41)

and

\[
\langle F^2(n) \rangle = \langle F^2(n-1) \rangle^{(K-1)d}(2^{K-1} - 1/2 + g(r_{n-1}))^d.
\] (42)

These expressions can be simplified a bit. We can write

\[
r_{n+1} = \left[\frac{(1 + r_n)^{K-1}}{\beta_K - 1 + (1 + r_n)^{K-1}}\right]^d
\] (43)
Table 1. The critical values of $d$ for the first and second moments on the rooted tree, determined by numerically solving the recursion relations derived in the text. The fourth column contains an estimate of the critical value from the expression for the second moment in equation (46).

| $K$ | $\langle F \rangle$ | $\langle F^2 \rangle$ | $\langle Z_o^2 \rangle$ |
|-----|---------------------|---------------------|---------------------|
| 2   | 2.41                | 3.06                | 2.9                 |
| 3   | 5.19                | 7.16                | 5.89                |
| 4   | 10.74               | 15.24               | 11.6                |
| 5   | 21.832              | 31.34               | 22.8                |
| 6   | 44.014              | 63.52               | 45                  |
| 7   | 88.376              | 127.86              | 89.5                |
| 8   | 177.099             | 256.51              | 177.6               |

defining $(2^{K-1} - 0.5)/(2^{K-1} - 1) \equiv \beta_K$ and

$$\langle F^2(n) \rangle = \langle F^2(n-1) \rangle^{(K-1)d} (2^{K-1} - 1)^{(K-1)d} \beta_K - 1 + (1 + r_{n-1})^{K-1} d.$$  (44)

Solving these numerically for different $K$, we get the numbers in the third column of table 1.

That different moments pick out different critical values of $d$ is not confined to the tree. We argue below that the $K$-SAT on a random graph, behaves similarly.

As mentioned earlier the behaviour of the first moment on the random graph is identical to that on a tree from simple considerations. The second moment, while not calculable in closed form for a random graph can be written in terms of the fraction of realizations that a pair of assignments are both simultaneously solutions of. The probability of two assignments simultaneously being a solution for a given realization depends on the overlap between the two assignments. If two assignments have an overlap $pN$ ($0 \leq p \leq 1$), the probability that both are solutions is $f(p)^M \equiv (1 - 2^{1-k} + 2^{-k} p^k)^M$ where $M$ is the total number of clauses. The exact expression for the second moment is thus simply the number of pairs of assignments with overlap $pN$ times the probability that such pairs are both simultaneously solutions for a realization [12,13].

$$\langle Z_o^2 \rangle = 2^N \sum_{z=0}^N \binom{N}{z} f(p = z/N).$$  (45)

Following Achlioptas et al [13] and using the leading-order approximation $\binom{N}{z} = (p^z(1-p)^{1-z})^{-N} \text{poly}(N)$, the term which contributes the maximum to the above sum is

$$2^N \left( \max_p \left[ \frac{f(p)^\alpha}{(p^z(1-p)^{1-z})} \right] \right)^N \text{poly}(N).$$  (46)

For our purposes it is easy to see, by plotting the term which is exponentiated in $N$ as a function of $p$, that there is a value of $\alpha$ above which the maximum value (which is an estimate of the second moment) is less than 1. The numbers at which this happens for different $K$ are reported in the fourth column of table 1. We have also estimated the critical value using simulations. For example, figure 3 plots the second moment as a function of $N$ for various values of $\alpha$ for random 3-SAT. We find that the value of $\alpha$ for which the second moment starts decaying with increasing $N$ is $5.7 \pm 0.1$. Hence, at least
for random 3-SAT, the value of the critical point for the second moment obtained from
the overlap function is close to the numerical estimate. Simulations for higher moments
near the critical point are harder to do since the fraction of successful realizations decays
exponentially with \(N\). For example, at \(\alpha = 5.7\) and \(N = 70\), only 208 out of the \(10^6\)
randomly chosen realizations had solutions. However, we expect the higher moments to
behave similarly, see for example [12] where expressions for the third and fourth moments
are also evaluated for random 3-SAT.

The quantitative differences in the values of the critical point for the second moment
in between our model and random \(K\)-SAT can be explained in terms of the boundary
conditions of the tree graph. For the tree graph, the probability that two assignments are
simultaneous solutions needs to be rewritten for the nodes near the boundary. If we make
the simple assumption that all nodes are nodes at depth 1, then we should replace \(f(p)\)
by \(g(p) = (1 - 2^{1-k} + 2^{-k}p)\) in the expression for the second moment in equation (46).

The critical values of \(d\) for the different moments, indicate the heterogeneity of dif-
ferent realizations. Even at very large values of \(d\) (or \(\alpha\)), there exist (an exponentially
rare number of) realizations which by having an exponentially large number of solutions,
contribute to the corresponding moment. The critical values for different moments also
provide bounds on the solvability transition. For example, the critical value for the first
moment gives a simple upper bound on the solvability transition for any \(K\). The ratio
of the square of the first moment to the second moment provides a lower bound on the
probability that solutions exist, and is the starting point for the weighted second moment
method [14]. However, to gain a better insight into the solvability transition, it is more
useful to look at how the fraction of solvable realizations changes as the number of con-
straints increases. This quantity can again be exactly calculated on a rooted tree and we
carry out this calculation in section 6.

6. Exact recursion relations on the tree for the probability that a variable can take
2, 1 or 0 values for arbitrary \(K\)

We would like to estimate the probability that a realization has no solution. Such a
realization is one for which not a single assignment of the variables provides a solution.
In this case there will be at least one unsatisfied clause if variable below, we describe how to set up the recursions for 2-SAT and then for a general $K$-SAT. The term $P_{n+1}(0)$ to be the probability that (or the fraction of realizations in which) a variable at depth $n$ can neither take the value 0 nor take the value 1, without causing a contradiction in its subtree. Note that because of the tree structure, all variables $x_i$ at depth $n$ will have the same probability $P_n$. The probability that a variable at depth $n$, can take only one of the two values 0 or 1 is defined to be $P_{n}(1)$. Similarly the probability that a variable at depth $n$ can take both values is $P_{n}(2) = 1 - P_{n}(0) - P_{n}(1)$. As before, in all that follows, we consider the boundary variables to have depth 0. In the sections below, we describe how to set up the recursions for 2-SAT and then for a general $K$-SAT.

We would like to calculate $P_{n+1}(0)$ and $P_{n+1}(1)$ for variable $x_0$ (assuming it is at depth $n+1$), given these quantities for its descendants. Let us consider $P_{n+1}(0)$ first for the 2-SAT problem. Assume variable 0 has a degree $d$ (by definition) and assume it is not negated on $d_1$ of these links. Variable $x_0$ will not be able to take the value 0 in the case when at least one of the $d_1$ links is not satisfied by the variable at the other end. In this case there will be at least one unsatisfied clause if variable $x_0$ takes the value 0. Similarly, at least one of the $d - d_1$ links along which variable $x_0$ is satisfying its link should also not be satisfied by the variable at the other end. This latter condition implies that variable $x_0$ cannot take the value 1 either. It is easy to see that averaging over all realizations at depth $n+1$ implies averaging over all values of $d_1$ as before, and averaging over all realizations at depth $n$. It is important to note, however, that all the realizations at depth $n+1$ are only built up from those realizations at depth $n$ that do have solutions.

Putting all this together the recursion relations for 2-SAT are:

$$P_{n+1}(0) = \sum_{d_1} \frac{1}{2^d} \left( \begin{array}{c} d \\ d_1 \end{array} \right) \left[ 1 - \left( 1 - \left( \frac{P_n(1)}{2(1-P_n(0))} \right) \right)^{d_1} \right]$$

$$\times \left[ 1 - \left( 1 - \left( \frac{P_n(1)}{2(1-P_n(0))} \right) \right)^{d-d_1} \right]$$

$$= 1 - 2 \left( 1 - 0.5 \left( \frac{P_n(1)}{2(1-P_n(0))} \right) \right)^d + \left( 1 - \left( \frac{P_n(1)}{2(1-P_n(0))} \right) \right)^d$$

$$P_{n+1}(1) = 2 \left( 1 - 0.5 \left( \frac{P_n(1)}{2(1-P_n(0))} \right) \right)^d - 2 \left( 1 - \left( \frac{P_n(1)}{2(1-P_n(0))} \right) \right)^d$$

The term $P_n(1)/(2(1-P_n(0))) \equiv Q_n(1)$ which appears in the above equations is just the conditional probability that a depth $n$ variable cannot satisfy its link above (to depth
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$n + 1$, given that it has to be able to take at least one value (which satisfies the subtree of which it is the root). The only way the latter can happen is if the one value it can take, does not satisfy the link above (this happens with probability $1/2$ in our case). If the variable can take two values, we can always find one value which satisfies the link above for any realization. We can iterate these equations beginning with the boundary conditions

$$P_1(1) = 2(0.75)^d - 2(0.5)^d \quad P_1(0) = 1 + (0.5)^d - 2(0.75)^d.$$  \hspace{1cm} (48)

The boundary conditions are easily obtained by setting $P_0(1) = 1$ in equations (47). We can hence obtain $P_n(0)$ for any depth $n$. The probability that a realization has a solution is then (as mentioned earlier) $\Pi_n(1 - P_n(0))^{g(n)}$ where $g(n)$ is simply the number of variables at depth $n$. If $P_n(0) \neq 0$ then the above product decays exponentially to 0 with increasing tree size. We see from equation (47) that it is when $P_n(1)$ takes a non-zero value that the fraction of realizations that have no solutions also becomes non-zero.

For a tree graph, since the boundary vertices form most of the graph, we can just take a look at equation (48). If we plot $P_1(0)$ as a function of $d$, we see immediately that this is non-zero for any $d > 1$ and hence the fraction of realizations that do not have solutions is non-zero above $d = 1$. This conclusion is true even if we calculate $\Pi_n(1 - P_n(0))^{g(n)}$ using the recursions and calculating $g(n)$, the number of vertices at depth $n$, for each depth. Hence for $d > 1$ the probability of having a realization with solutions goes down exponentially with $N$. For example, for $d = 3$, $K = 2$ and $n = 4$, we find from exact enumerations, that out of $10^7$ randomly generated instances, only 77 have solutions. Note, however, that these 77 suffice to make the second and higher moments still an increasing function of $N$, as we saw in the previous section.

The recursion relations for 2-SAT are easily generalized to arbitrary $K$.

$$P_{n+1}(0) = 1 - 2(1 - 0.5(Q_n(1))^{K-1})^d + (1 - (Q_n(1))^{K-1})^d$$

$$P_{n+1}(1) = 2(1 - 0.5(Q_n(1))^{K-1})^d - 2(1 - (Q_n(1))^{K-1})^d \hspace{1cm} (49)$$

with the boundary conditions obtained by putting $P_0(0) = 0$ and $P_0(1) = 1$ as before.

We find that for all $K$, for $d > 1$, the fraction of realizations that have solutions decays exponentially with $N$. Since this is also usually how the SAT–UNSAT transition is defined numerically, we can conclude that $\Pi_n(1 - P_n(0))^{g(n)}$ is the order parameter for the solvability transition in our model. The transition occurs at $d = 1$ for all $K$ when the boundaries are fixed randomly. In comparison, for random 3-SAT the value of $\alpha$ (that we find from simulations) at which the fraction of successful realizations starts decaying exponentially is $\alpha = 4.25 \pm 0.05$. Hence both the behaviour of the moments, as well as the SAT–UNSAT transition, is qualitatively similar to random $K$-SAT, though quantitatively, on the tree graph, these are influenced mostly by the surface variables, as expected. Hence in section 7, we look at the behaviour of equations (47) and (49) in the interior of the tree, for an infinite rooted tree.

7. Fixed point analysis

In this section we will try to get rid of boundary effects by looking deep within the tree. This is usually equivalent to doing a calculation on a Bethe lattice, in which case, all vertices on the tree should be equivalent and have the same coordination number.
On the rooted tree we have discussed so far, the root has a coordination number 1 less than the other sites. However, from the structure of the recursions equation (49), for any vertex/variable on the tree, it is only $d$ of the connections (to descendants) which determines the probability $P_n(0)$. Hence $P_n(0)$ at a depth $n$ is not changed when more levels are added to the tree. The same is not true for $P_n(1)$ which, at least when $P_n(0) \neq 0$, needs to be corrected, for interior sites. However, this correction does not affect the transition that we discuss below. We can hence hope that the fixed point of the recursions equations (47) and (49) will give us an insight into how these probabilities behave in the interior of the tree, independent of boundary conditions.

Consider the recursions (equation (47)) for 2-SAT first. Noticing that it is the quantity $Q_n(1)$ which appears on the RHS of these equations, we can rewrite the recursions as

$$Q_{n+1}(1) = \frac{[1 - 0.5Q_n(1)]^d - [1 - Q_n(1)]^d}{2[1 - 0.5Q_n(1)]^d - [1 - Q_n(1)]^d} \tag{50}$$

If the above map has a fixed point, then the value of $Q_n(1) = Q_{n+1}(1) = Q^*$ and $Q^* = f(Q^*)$ where $f(Q^*)$ is the function on the RHS and $0 < Q^* < 1$.

We can look for this graphically as shown in figure 4. For $d < 2$, there is only one solution to the equation $Q^* = f(Q^*)$ and this lies at $Q^* = 0$. For $d > 2$ there are two solutions, one at $Q^* = 0$ and the other at some non-zero $Q^*$. If $Q^* = 0$, clearly $P_n(0) = 0$, for large $n$. This implies that (assuming all $N$ nodes in our system are deep in the tree), the probability that a realization has a solution (sequence $1-P(0)$) is 1. Equivalently if $Q^* \neq 0$, this probability vanishes as $N \to \infty$. Note that the non-zero value of $Q^*$ develops continuously from $Q^* = 0$. In other words, for $d$ only very slightly larger than 2, the non-trivial solution is only very slightly larger than 0. In addition, from the shape of the function $f(Q^*)$ we see that no matter what the boundary conditions, the non-trivial fixed point is always reached for $d > 2$. Hence for 2-SAT, in the interior of an infinite tree, a real transition (the solvability transition) occurs at $d = 2$. 

Figure 4. Fixed points for $d < 2$ and $d > 2$ for 2-SAT.
On general grounds [15], we expect that the above results are comparable with those on a regular random graph with coordination number $\alpha = (d + 1)/2$ and hence a transition at $d = 2$ in the interior of a tree should correspond to $\alpha_c = 1.5$. It is interesting to note, however, that if we use instead the relation $\alpha = d/2$ (as used in the correspondence between the cavity method and tree reconstruction) this gives the solvability transition for random 2-SAT to lie at $\alpha = 1$ which is an exact and known result.

Consider the case $K > 2$ now. As before, we can write

$$Q_{n+1}(1) = \frac{[1 - 0.5Q_n(1)^{K-1}]^d - [1 - Q_n(1)^{K-1}]^d}{2[1 - 0.5Q_n(1)^{K-1}]^d - [1 - Q_n(1)^{K-1}]^d}. \tag{51}$$

We can investigate the fixed points graphically as shown for $K = 3$ in figure 5. For $d < 11.5$, there is only one solution to the equation $Q^* = f(Q^*)$ and this lies at $Q^* = 0$ as before. For $d > 11.5$ there are three solutions, one at $Q^* = 0$ and the other two at some non-zero $Q^*$.

Some important points of difference with 2-SAT are that the non-zero values of $Q^*$ develop discontinuously from $Q^* = 0$. Also, from the shape of the function $f(Q^*)$, the first ($Q^* = 0$) and third (non-trivial) value of $Q^*$ are stable while the middle value is unstable. This is true for all $K \geq 3$. Hence from the shape of the function $f(Q^*)$ we also see that boundary conditions play an important role for $K > 2$. The non-trivial solution is reached only if the boundary conditions are such as to make the value $Q_0(1)$ larger than the value of the central fixed point. This points to a first-order transition for $K \geq 3$ as opposed to a continuous transition for $K = 2$. This difference in the nature of the transitions at $K = 2$ and $K > 2$ is entirely analogous to the problem on a random graph [16].

For $K > 2$ the correspondence between the average degree of a variable on a regular random graph and that of a variable on the tree comes out to be $\alpha = (d + 1)/K$.

In table 2 we report the value $d_c$ as obtained from the fixed point equations for our model, as well as both $(d_c + 1)/K$ and $d_c/K$. It is interesting to note that these latter values are very close to the value of $\alpha_d$ obtained in the literature earlier [8,17].
Table 2. The value of $d_c$ compared to $\alpha_d$ values obtained from [8].

| $K$ | $d_c$ | $(d_c + 1)/K$ | $d_c/K$ | $\alpha_d$ (from [8]) |
|-----|-------|--------------|---------|---------------------|
| 2   | 2     | 1.5          | 1       | 1                   |
| 3   | 11.5  | 4.166        | 3.83    | 3.927               |
| 4   | 32.6  | 8.4          | 8.15    | 8.297               |
| 5   | 80    | 16.2         | 16.00   | 16.12               |
| 6   | 182   | 30.5         | 30.33   | 30.5                |
| 7   | 400   | 57.28        | 57.14   | 57.22               |
| 8   | 856   | 107.13       | 107.00  | 107.24              |

Note that in our case the value $d_c$ appears as that value of $d$ in the interior of an infinite tree from which point onwards a solvability transition could take place, depending on the boundary values. It is only for 2-SAT that the transition actually does coincide with $d$ taking the value $d_c$.

8. Summary and discussion

In this paper, we have studied the $K$-SAT problem on a rooted tree and have solved it exactly for several quantities. A lot of progress in understanding the $K$-SAT problem has been made using the cavity method [7, 8, 22] and a powerful heuristic, survey propagation (SP) [22, 23] has been developed using these concepts. The SP equations, which are the basis for the algorithm, are a set of coupled equations for the cavity bias surveys—messages sent from clauses to variables—in terms of the probabilities of warnings received by the variable. The probability space over which these are computed is the space built by all SAT assignments each given equal probability in a typical satisfiable instance. It is conjectured that this solution space, for $\alpha > \alpha_d$, separates into many distant clusters, and hence the SP message along an edge gives the probability that a warning is sent in a randomly chosen cluster. Under this assumption, the SP equations lead to coupled integral equations with a non-trivial fixed point, known as the ‘one step RSB’ solution. The same fixed point equations may also be obtained by different means, by considering a reconstruction problem on a tree [9]. The difference between a RS (replica-symmetric) solution and a 1RSB solution in the tree case, is due to the absence or presence of a re-weighting factor in the fixed point equation [9]. This re-weighting factor may be thought of as the term in equations (1) and (2), for example, which involves the $\eta$s. Were we to replace the $\eta$s simply by $1/2$ (their average value), then the recursion would give the number of solutions at the next level of the tree as simply the product over the previous level. The presence of the $\eta$s makes the recursion more non-trivial. The recursions in sections 6 and 7, too, keep this re-weighting factor.

Another difference in our work from the cavity method or SP is that the marginal probabilities are calculated level by level, instead of for each variable separately. This simplifies analysis, but makes our treatment valid strictly only for trees, unlike SP which is used to solve the SAT problem also on random graphs (though there are no guarantees of convergence in this case).

Our model shows many of the non-trivial features of the full random $K$-SAT problem. To summarize, we find that different moments of the number of solutions start to decay...
at different values of $d$. These values of $d$ are much larger than the value at which the solvability transition occurs. Also the solvability transition in our model is continuous for $K = 2$ and discontinuous for $K > 2$, as in random $K$-SAT. In addition the fixed point equations predict for $K > 2$, a lower bound on the solvability transition in the interior of the tree. These numbers if converted to equivalent $\alpha$ values on the random graph are very close to the values predicted for $\alpha_d$ in the literature for random graphs with an average node-degree $K\alpha$ (to make a more literal correspondence to our tree where every variable has the same degree, it would be interesting to compare with $\alpha_d$ values predicted for regular random graphs). We should note though that the existence of $\alpha_d$ is motivated in the literature by the structure of the space of solutions in random $K$-SAT, while in this work it arises as the point at which the recursions can have more than one solution, depending on boundary conditions. At this point, the fraction of realizations in which a variable is constrained to take the same value in all SAT assignments becomes non-zero.

We can redo the computation of equations (49) as well as the fixed point analysis for other variations of the SAT problem such as regular random $K$-SAT, introduced in [18] and for which bounds on the threshold are derived in [19]. Preliminary results from the fixed point analysis show that the fixed point equations have a similar behaviour as for $K$-SAT, but predict smaller values of $d_c$ for the same $K$ [20], as indeed is also the numerical prediction for the solvability transition for this problem [18]. It should also be possible to redo these calculations on a random tree (where the degree of each vertex is Poisson-distributed), though we do not expect the results to change qualitatively in this case. Another interesting generalization of these calculations is to compute a more fine-grained quantity than $P_n(2)$, namely to compute the probability that the root takes one of the two values a certain fraction $\beta$ of the times. It would be interesting to see if this quantity undergoes a transition in which $\beta$ changes from essentially taking the value 1/2 to having a non-trivial distribution. Note that a similar calculation for random tree ensembles, with, however, an average done over boundary conditions chosen uniformly over all satisfying assignments, is done in [21].

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