Ground state of the Bethe-lattice spin glass and running time of an exact optimization algorithm
EXTENDED ABSTRACT

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In this talk, we present results from our study Ref. 1 where we analyze Ising spin glasses on random
graphs with fixed connectivity z and with a Gaussian distribution of the couplings, with mean μ
and unit variance. We compute exact ground states by using a branch-and-cut method for z = 4, 6
and system sizes up to 1280 spins, for different values of μ. We locate the spin-glass/ferromagnet
phase transition as μ = 0.77 ± 0.02 (z = 4) and μ = 0.56 ± 0.02 (z = 6). We also compute the energy
and magnetization in the Bethe-Fejér’s approximation with a stochastic method, and estimate the
magnitude of replica symmetry breaking corrections. Near the phase transition, we observe a sharp
change of the median running time of our implementation of the algorithm, consistent with a change
from a polynomial dependence on the system size, deep in the ferromagnetic phase, to slower than
polynomial in the spin-glass phase.

I. INTRODUCTION

Recent years have seen an increasing interaction be-
tween the fields of combinatorial optimization and sta-
tistical physics5–8. On one hand, several problems in
the statistical physics of disordered systems have been
mapped onto combinatorial problems, for which fast
combinatorial optimization algorithms are available9–10.
This has provided valuable insights into questions that are
hard to investigate with traditional techniques, such as
Monte Carlo simulations. On the other hand, concepts and
methods from statistical physics are increasingly ap-
plied to combinatorial optimization8.

Easy/hard thresholds analogous to phase transitions
have been observed in random instances of optimization
and decision problems, including satisfiability (SAT)7,8,
vertex-cover2 (VC), number partitioning11, and others.
There is currently much interest in understanding how
phase transitions affect the performance of combina-
torial algorithms, following the observation12 that the
average12 or typical (i.e. median) running time of some
algorithms exhibits a sharp change in the vicinity of a
phase transition. (Note, however, that from the behav-
or of individual algorithms, strictly speaking, one cannot
draw conclusions about the “typical hardness” of a prob-
lem itself). Recently, statistical physics techniques have
been fruitfully applied to study easy/hard transitions and
algorithmic performance6.

Here, we apply a branch-and-cut algorithm, a tech-
nique developed in combinatorial optimization, to find
the ground state of the Ising spin glass on random
graphs with fixed coordination number (also called Bethe
lattices). Our first goal is algorithmic: we want to
characterize the typical running time of our algorithm,
notably its behavior across the zero-temperature spin-
glass/ferromagnet phase transition that occurs when
varying the mean of the random couplings. The interest
of this stems from the importance of branch-and-cut as
a general technique in combinatorial optimization, and
from the fact that finding the ground state of a spin
glass is a prominent example of a hard optimization prob-
lem arising from statistical physics (in general, it is NP-
hard15).

The second motivation for the present work lies in the
ground-state properties of the Bethe-lattice spin glass,
which recently have attracted a renewed interest18–21. In
this talk, we first introduce the Bethe-lattice spin glass
model. We then describe the branch-and-cut algorithm
used to calculate the exact ground states of the model.
We describe the Bethe-Fejér’s approximation and the
stochastic procedure used to solve it. We present our
branch-and-cut and BP results for the ground state en-
ergy and the zero temperature phase transition. We show
that this transition coincides with a change of the typical
running time.

II. MODEL

The system considered consists of N Ising spins $S_i = ±1$
sitting on the nodes of a graph $G = (V, E)$, where
$V = \{1, \ldots, N\}$ is the set of nodes and $E = \{(i, j)\} \subset
V \times V$ is the set of edges of the graph. The energy of
the system is given by

$$\mathcal{H} = -\sum_{(i,j) \in E} J_{ij} S_i S_j$$

(1)

where the couplings $J_{ij}$ are independent, identically dis-
tributed random variables drawn from a Gaussian distri-
bution $P(\cdot)$ with mean $\mu$ and unit variance,

$$P(J) = \frac{1}{\sqrt{2\pi}} \exp[-(J - \mu)^2/2]$$

(2)
We consider the case in which $G$ is a random graph with fixed connectivity $z$, or $z$-regular graph, where each spin interacts with exactly $z$ neighbors. This provides a convenient realization of a Bethe lattice.9,18 Frustration is induced by large loops, the typical size of a loop being of order $\log N$. Small loops are rare, giving the graph a local tree-like structure, and therefore the mean field approximation is exact.

Although it has long been known that replica symmetry is broken in these two models,9–11,22–24, until recently a replica symmetry broken solution could be found only in some limit cases. Mézard and Parisi recently introduced18,19 a “population dynamics” algorithm which allows a full numerical solution at the level of one step of replica symmetry breaking. Explicit results were derived for the Bethe-lattice spin glass with the symmetric $\pm J$ disorder distribution, but not for the Gaussian distribution considered here or for a non-zero mean. Previous numerical studies of this model can be found in Refs. 21, 25, 26. For a complete discussion of the Bethe-lattice spin glass, see Ref. 18 and references therein.

III. BRANCH-AND-CUT ALGORITHM AND BP RECURSION

The problem of finding a ground state of the Hamiltonian in Eq. (1) is in general computationally demanding. For a generic graph $G$, it is NP-hard.8,15 For NP-hard problems, currently only algorithms are available, for which the running time increases faster than any polynomial in the system size, in the worst case. In the special case of a planar system without magnetic field, e.g. a square lattice with periodic boundary conditions in at most one direction, efficient polynomial-time matching algorithms27 exist. For the square lattice with periodic boundaries in both directions, polynomial algorithms exist for computing the complete partition function for the $\pm J$ distribution28 and for the case in which the coupling strengths are bounded by a polynomial in the system size29. In practice, both algorithms can only reach relatively small system sizes.

For the Bethe lattice considered here (and for regular lattices in dimension higher than two), no polynomial algorithm is known. We study the branch-and-cut method16,30,35 (see Ref. 31 for a tutorial on optimization problems and techniques, including branch-and-bound and branch-and-cut), which is currently the fastest exact algorithm for computing spin glass ground states17, with the exception of the polynomial-time special cases mentioned above. In the talk we will explain more details about the algorithm; see also Ref. 1.

Here, for solving the BP recursion, we employ the stochastic iterative procedure proposed by Mézard and Parisi19 for the more general one-step replica symmetry broken case (see also Ref. 24 for a previous application of a similar method), see Ref. 1 for details. The BP recursion, especially at finite temperature, has been studied extensively (see Ref. 18 and references therein). In particular, Mézard and Parisi19 have given an analytic expression of $P(h)$ for a binary $P(J)$.

IV. RESULTS

We have studied the Ising spin glass on random graphs with fixed connectivity $z = 4$ and $z = 6$. The instance generator first builds a random regular graph with the algorithm described in Ref. 34. We then assign the couplings $J_{ij}$ according to the distribution $P(J)$ in Eq. (2).

Using the branch-and-cut approach we were able to study graph sizes up to $N = 400$ for $z = 4$ and $\mu \leq 0.9$, and up to $N = 200$ for $z = 6$ and $\mu \leq 0.7$. For larger values of $\mu$, we considered sizes up to $N = 1280$. Incidentally, for Ising spin glasses on a regular grid, specialized heuristics exist that exploit the grid structure, making it possible to consider larger system sizes than for the model reported here.

The largest number of samples were considered in the vicinity of the phase transition, where the fluctuations of the magnetization are larger. Near the transition, for sizes $N \leq 240$ ($z = 4$) and $N \leq 100$ ($z = 6$) we computed around 5000 samples for each value of $\mu$; for $N = 400$ ($z = 4$) and $N = 200$ ($z = 6$), around 500 samples for each value of $\mu$. For sizes larger than these, we computed up to 250 samples for each $\mu$. In the following analysis of the ground state energy and magnetization, we consider only sizes up to $N = 400$ ($z = 4$) and $N = 200$ ($z = 6$), since for larger sizes the statistical error is quite large. In the analysis of running times we will include all sizes.

A. Ground state energy

We start by showing, in Fig. 1, the average ground state energy $E(\mu, N)$, divided by $zN$, as a function of $\mu$ for $z = 4, 6$ and two different system sizes. For sufficiently large $\mu$, the system is completely magnetized, therefore the ground state energy depends linearly on $\mu$, $E(\mu, N)/N \sim \rho \mu$, as visible in the figure. For small $\mu$ the system is frustrated, hence the energy saturates. The lines in Fig. 1 represent the numerical solution of the BP recursion obtained with a population size $N' = 10^6$ (we verified that with $N' = 10^7$ the results are unchanged) and $M = 10^4$ iterations of the stochastic algorithm. Clearly, the branch-and-cut results agree well with the BP approximation.

We extrapolate the branch-and-cut results to $N = \infty$ by fitting the data with the form $E/N = e_{\infty} + bN^{-2/3}$. As shown in Fig. 2, the finite size corrections are well described by a $N^{-2/3}$ dependence for small $\mu$, although an $N^{-1/3}$ correction fits reasonably well the data for other values of $\omega$ between 0.6 and 1 as well. For large $\mu$, the finite size corrections are very small. A $N^{-2/3}$ correction was also found to fit well the numerical data by Boettcher21,
who computed the average ground state energy of the \( \pm J \) model for \( z \) up to \( z = 26 \) and \( N \) up to \( N = 2048 \) using a heuristic algorithm. In Ref. 18, the finite-size dependence of the energy at \( T = 0.8 \) was studied, for the \( \pm J \) distribution and \( z = 6 \), finding a finite-size exponent \( \omega = 0.767(8) \), not far from 2/3.

Fig. 2 also shows that the extrapolated energy, \( e_\infty \), is very close to the BP result, \( e_{BP} \), in the whole range of \( \mu \). Of course, the agreement is not surprising for large \( \mu \), where replica symmetry holds. For smaller \( \mu \), the observed agreement indicates that replica symmetry breaking corrections to the ground state energy are small (less than 1%).

In particular, for \( \mu = 0 \) we obtain \( e_\infty = -1.38 \pm 0.04 \) (\( z = 4 \)) and \( e_\infty = -1.72 \pm 0.02 \) (\( z = 6 \)), where the errors take into account the uncertainty on the correction exponent \( \omega \), to be compared with our BP result \( e_{BP} = -1.351 \pm 0.002 \) (\( z = 4 \)) and \( e_{BP} = -1.737 \pm 0.002 \) (\( z = 6 \)).

**B. Ground state magnetization**

In the following we present both for the BP recursion and the branch and cut data the results for the average ground state magnetization \( m = \langle M \rangle \), where \( M = \frac{1}{N} \sum_s S \cdot S_0 \) and \( \langle ... \rangle \) denotes the sample average, as a function of \( \mu \) for different system sizes \( N \). An estimate of the critical coupling strength \( \mu_c \) can be obtained from

\[
g(\mu) = \frac{1}{2} \left( 3 - \frac{[M^4]}{[M^2]^2} \right),
\]

where for the BP recursion \( \langle ... \rangle \) is the “time” average. In the limit \( N \to \infty \), \( g(\mu) = 0 \) for \( \mu < \mu_c \) and \( g(\mu) = 1 \) for \( \mu > \mu_c \), hence \( g(\mu) \) can be used to locate \( \mu_c \). As shown in Fig. 3, the variation of the Binder cumulant with \( \mu \) sharpens as \( N \) increases, an effect of the sign oscillations of the magnetization, which become less important as \( N \) increases. From \( N = 10^5 \) we estimate

\[
\mu_{BP}^c = 0.743 \pm 0.005 \quad (z = 4)
\]

\[
\mu_{BP}^c = 0.547 \pm 0.005 \quad (z = 6)
\]

We verified that with these values of \( \mu_c \), the magnetization obeys \( m_{BP} = d(\mu - \mu_c)^\beta \) for \( \mu \approx \mu_c \), with the mean-field exponent \( \beta = 1/2 \) and \( \alpha \approx 0.23 \).

Klein et al.\(^{35}\) solved the BP recursion in the vicinity of \( \mu_c \), using the mean random field approximation (MRF). Their results \( \mu_{BP}^{MRF} = 0.775 \) (\( z = 4 \)) and \( \mu_{BP}^{MRF} = 0.587 \) (\( z = 6 \)) (obtained after rescaling their value by an appropriate normalization factor \( \sqrt{\pi} \)) are slightly larger than our result \( \mu_{BP}^c \).

In order to obtain an estimate of \( \mu_c \), from the finite-\( N \) branch-and-cut data, we computed the Binder cumulant \( g(\mu, N) \), defined as in Eq. (3) but with the time average replaced by the sample average. According to finite-size scaling, the curves for \( g(\mu, N) \) as a function of \( \mu \) for various \( N \) must cross at the critical point \( \mu = \mu_c \). In Fig. 4 we plot the Binder cumulant in the vicinity of the intersection point (note that the horizontal scale is much
Fig. 3: Binder cumulant from the stochastic solution of the BP ansatz, for three different sizes of the stochastic population $N$. Corrections shift $\mu_c$ from 1.25 to 1. Although our numerical estimate of $\mu_c$ is slightly larger than $\mu_c^{BP}$ instead, this could be a statistical fluctuation or a finite-size effect.

The Binder cumulant is expected to satisfy the following finite-size scaling relation $^{36}$ for $\mu \approx \mu_c$:

$$g(\mu, N) = \tilde{g}(N^{1/(d_w \nu)} (\mu - \mu_c))$$

where $d_w$ is the upper critical dimension, which for the Ising spin glass is $d_w = 6$. As usual, by plotting $g(\mu, N)$ against $N^{1/(d_w \nu)} (\mu - \mu_c)$ with correct parameters $\mu_c$ and $\nu$, the data points for different system sizes should collapse onto a single curve near $(\mu - \mu_c) = 0$. As shown in Fig. 5, using the estimates of $\mu_c$ obtained above and the mean-field exponent $\nu = 1/2$ we obtain a good data collapse, showing that finite size scaling is well satisfied in our range of sizes.

V. TYPICAL RUNNING TIME OF OUR BRANCH AND CUT ALGORITHM

In the following we study the running time of our program as a function of the mean coupling strength $\mu$. In practice, the running time can vary greatly from an instance of the problem to another, and the worst-case running time might very rarely occur. Recent work has therefore focused on the average running time with respect to random instances drawn from some probability distribution. Instead of the average one can also analyze the median, or typical running time, which has the advantage of being less influenced by the occurrence of exponentially rare samples with huge running times.

It should be noted that, unlike the usual worst-case complexity classification, which is an algorithm-
are bending upwards, indicating that the running time increases faster than any polynomial. This is also the case for \( \mu = 0.8 \) (\( z = 4 \)) and for \( \mu = 0.6 \) (\( z = 6 \), not shown).

Hence from this data, it seems that the change in the typical running time occurs at a value of \( \mu \) larger than \( \mu_c \), although it is difficult to locate a precise transition point.

We have fitted the data in Fig. 7 with a function of the form \( n_{\text{ps}}(N) \sim \exp(bN^\zeta) \). For \( \mu = 0 \), we find \( b = 0.026(9) \), \( c = 0.87(5) \) for \( z = 4 \), and \( b = 0.007(3) \) and \( c = 1.24(8) \) for \( z = 6 \), but the data exhibits in both cases a considerable scatter around the fitting region, prohibiting to conclude in a definite way that the typical running time is exponential. Nevertheless, the data strongly suggest so.

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\[\text{[1] F. Liers, M. Palassini, A.K. Hartmann, M. Jünger, cond-mat/0211630}\]
[12] In the computer science literature, the term average-case running time is usually employed.