An interior point cutting plane algorithm for Ising spin glass problems

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Abstract

An interior point cutting plane algorithm for solving Maximum Cut problems of a particular structure is described. The problem of interest is determining the ground states of two dimensional $\pm J$ Ising spin glasses on square lattices with nearest neighbour interactions and periodic boundary conditions. Computational results for grids of sizes up to 100×100 are presented. An estimate of the ground state energy of an infinite spin glass system with the proportion of negative bonds equal to 0.5 is given.

1 Introduction

This paper describes an approach to a problem in glassy dynamics in statistical physics. An *Ising spin glass* is a model of a magnetic material, and it consists of a grid of magnetic spins. Each spin S_i is in one of two states, which we call "up" and "down"; we assign S_i the value $+1$ if the spin is up and -1 if the spin is down. In this paper, we assume the grid is an $L \times L$ square grid embedded on a torus. Further, we assume that the interactions between spins are restricted to neighbours, that is, we consider the short range model with Ising spins S_i. At very low temperatures, the spin glass will be in its *ground state*, or state of lowest energy; it is this state that we wish to determine. Thus, given the interactions J_{ij} between neighbouring spins, the objective is to determine the directions of the spins that minimizes the total energy E. This can be calculated by minimizing the Hamiltonian H of the energy:

$$H = - \sum_{\text{neighbours } i,j} J_{ij} S_i S_j. \tag{1}$$

We consider the case where all interactions J_{ij} are restricted to take the same magnitude J, but the sign is random; we took $|J| = 1$. The principal properties of real spin glasses (for example, amorphous alloys) are represented well by the $\pm J$ spin glass model on a rectangular lattice.

This problem was originally discussed in the optimization literature by Grötschel *et al.* [7, 1]; some of these authors have recently revisited this problem [4]. They proposed a branch and cut approach for this problem, using the simplex method to solve the relaxations. The hardest instances for their algorithm were where the interactions were equally likely to be ± 1; they were able to solve such instances with $L = 70$ in about a day of computation on a Sun SPARCstation 10. We consider using an interior point method to solve the relaxations; we are able to solve problems with $L = 100$ in an average of less than four hours on a Sun SPARCstation 20/71, and problems with $L = 70$ take approximately half an hour. We describe our algorithm in section 2. Our computational results are given in section 3.

We now describe the approach of [7, 1, 4] in more detail. The problem can be modelled on an undirected graph $G = (V, E)$ as

$$\begin{array}{lll} \min & \sum_{i=1}^{p} \sum_{j>i,(i,j)\in G} c_{ij} x_{ij} & (MC) \\ \text{subject to} & x \quad \text{is the incidence vector of a cut} & \end{array}$$

where p is the number of vertices, there is a binary variable x_{ij} for each edge, and the cost c_{ij} of each edge is derived from the interaction between the vertices. The optimal solution to this problem gives the ground state, with vertices on one side of the cut being up and vertices on the other side being down. The ground state energy can be calculated from the optimal value of (MC) in a simple manner. Each vertex has four neighbours, so a $k \times k$ grid will have k^2 vertices and $2k^2$ edges. It should be noted that the optimal value of (MC) will be even under the assumption that $| J_{ij} |= 1$ for all edge interactions [11].

Cutting planes can be derived by using the observation that every cycle and every cut intersect in an even number of edges. Every subset F of odd cardinality of every chordless cycle C gives the facet-defining inequality

$$x(F) - x(C \setminus F) \leq | F | - 1 \qquad (2)$$

where $x(S)$ denotes $\sum_{(i,j)\in S} x_{ij}$ for any subset $S \subseteq E$. The cycles of length four (the *squares*) in the graph are chordless cycles, and there are many other chordless cycles. There are other families of facet defining inequalities (see [2, 5, 6], for example); for Ising spin glass problems, facets of the form (2) were usually sufficient, and we only searched for such facets.

An alternative optimization approach to the maximum cut problem is to use semidefinite programming (SDP) [8]. Such an approach would work directly with equation (1) and set up one variable for each vertex. Computationally, the SDP approach works very well for graphs with up to about 100 vertices and the approach works equally well on dense graphs as on sparse graphs. However, for the Ising spin glass problem, the graph is very sparse, with each vertex having only four neighbours, and the SDP approach is not able to exploit this sparsity, so it is not competitive with the integer linear programming approach described in this paper for problems of the size in which we are interested.

2 An interior point cutting plane algorithm

The algorithm takes an initial relaxation consisting of the objective function given in (MC), along with the trivial bounds $0 \leq x \leq e$ (here, e denotes the vector of ones of appropriate dimension). This linear programming relaxation is solved approximately, using a primal-dual predictor-corrector interior point method (see, for example, [9, 10]). A heuristic cut is generated using this approximately optimal LP solution $\hat{x}$. The value of the relaxation provides a lower bound on the optimal value of (MC), and the best heuristic solution found so far provides an upper bound. If the gap between these two bounds is less than two then the best heuristic solution is optimal; otherwise, valid inequalities for (MC) that are violated by $\hat{x}$ are generated, the relaxation is modified, and the process is repeated.

There are several important aspects of this algorithm that require careful selection. The degree of accuracy required in the solution of the relaxations is gradually tightened, depending on the progress of the algorithm. If it appears likely that the solution to the current relaxation will enable the algorithm to terminate, then the algorithm continues to work on the current relaxation. The heuristic solution is generated using an exchange heuristic: the algorithm looks for chains of vertices that can be switched beneficially from one side of the cut to the other. The algorithm is restarted by setting the primal solution to be a convex combination of $0.5e$ and the approximate solution to the relaxation, and setting the dual solution to be an earlier dual point. The new primal point is chosen to be feasible in the new relaxation; the new dual point is also feasible, if the additional dual variables corresponding to the added primal constraints are set appropriately. The interested reader is referred to [11] for a more detailed discussion of the algorithm.

3 Computational results

The algorithm was implemented in FORTRAN 77 and all computational tests were performed on a Sun SPARC 20/71 UNIX workstation running SunOS. Grid sizes up to 100×100 were solved. One hundred problems of each grid width $L = 10, 20, ..., 90, 100$ were successfully solved.

It was not possible to solve approximately 5 problems using our implementation — either the relaxations became too large or the problems required additional inequalities of a different form from (2). For each of these problems, the gap between the upper and lower bounds was less than four when the algorithm terminated. In the calculations below, we omit the results for these problems. It should be noted that we repeated the calculations in section 3.1 with the inclusion of these unfinished runs, both with the energy of each of the unfinished runs taking its high value and also with the energy of each unfinished run taking its low value. The estimates for the ground state energy of an infinite grid were unchanged to six significant digits.

3.1 Energy estimates

The ground state energy was calculated for each of the successfully solved instances, and the results are contained in table 1. Note that the mean and variability of the ground state energy both decrease as the grid width increases.

L	Sample Size	Mean	Std Dev	Minimum	Maximum
10	100	-1.3946	0.0504	-1.5400	-1.2800
20	100	-1.3951	0.0216	-1.4550	-1.3400
30	100	-1.4013	0.0159	-1.4378	-1.3600
40	100	-1.3981	0.0110	-1.4276	-1.3700
50	100	-1.4000	0.0106	-1.4264	-1.3760
60	100	-1.4017	0.0075	-1.4194	-1.3783
70	100	-1.4014	0.0062	-1.4143	-1.3849
80	100	-1.4012	0.0062	-1.4163	-1.3888
90	100	-1.4020	0.0042	-1.4119	-1.3916
100	100	-1.4024	0.0048	-1.4134	-1.3864

Table 1: Ground state energy of Ising spin glass problems

The energy E was first modeled as

$$E_e(L) = E_e^\infty + ce^{-aL} \tag{3}$$

The least squares estimate for the ground state energy of an infinite grid was $E_e^\infty = -1.4004 \pm 0.0007$ and the appropriate F-test was significant at the 1 in 200 level. The proportion of error accounted for by the model, R^2, was very small, because of the high variability in the ground state energies for each gridsize.

We also analyzed the data using the quadratic model

$$E_q(L) = E_q^\infty + cL^{-2} \tag{4}$$

The least squares estimate given by this model was $E_q^\infty = -1.4009 \pm 0.0007$, significant at the 1 in 2000 level. The R^2 value for this model was slightly larger than that for the model in equation (3), but still very small. Note that the two estimates agree with each other, and they also both agree with the estimate of E_e^∞ given in [4].

We then repeated the analysis, but using just the runs with the grid width at least 70. This provided estimates for the ground state energy of $E_e^\infty = -1.4019 \pm 0.0003$ and $E_q^\infty = -1.4033 \pm 0.0011$. These estimates are noticeably smaller than the estimates given by the complete data set, indicating that the ground state energy may decrease more quickly as a function of gridsize than suggested by either model.

3.2 The time taken by the algorithm

The times required in seconds by the algorithm are given in table 2. It should be noted that the mean time to solve a problem with a grid width of 100 is only 3.5 hours, and the maximum time for such a problem was approximately six hours. This

L	Sample Size	Mean	Std Dev	Minimum	Maximum
10	100	0.42	0.20	0.17	1.17
20	100	4.87	2.01	1.30	12.48
30	100	24.32	11.84	7.42	87.00
40	100	88.46	43.68	32.50	259.02
50	100	272.86	151.59	96.35	795.50
60	100	860.57	969.79	227.38	7450.18
70	100	1946.14	1286.13	593.57	8370.37
80	100	5504.11	4981.00	1403.27	32470.40
90	100	10984.82	6683.37	2474.20	28785.30
100	100	12030.69	3879.55	3855.02	21922.60

Table 2: Time (seconds) to solve Ising spin glass problems

compares very favourably with the results in [4], where problems with a grid width of 70 took approximately one day, using the simplex solver in CPLEX 3.0 [3].

The linear programming relaxations of the largest problems have 20000 variables and approximately 11000 constraints at termination, a size where an interior point method can be expected to outperform an implementation of the simplex algorithm.

We constructed a model of the form

$$\log_e(time) = c + m \log_e(L) \tag{5}$$

The least squares estimate for m was 4.64 ± 0.02, significant at the 1 in 10000 level, and this model had an R^2 of 96%. The model indicates that the runtime grows approximately at the rate $L^{4.6}$. This contrasts with [4], where the runtime appeared to grow at L^6. Such a result is not surprising for an interior point algorithm.

4 Conclusions

We have demonstrated that the use of an interior point cutting plane algorithm makes it possible to calculate the ground states of Ising spin glasses of sizes larger than previously possible. This has made it possible to calculate new estimates of the ground state energy of an infinite spin glass.

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