Computing for the Physical and Social Sciences (COS 323) – Fall 2001

Assignment 4: Ground States of Ising Spin Glasses (W. Cook)
Due Date: December 11, in class

Many successful models in physics depend on the orderly nature of matter; the order permits simplifying assumptions that allow the models to be attacked with elegant mathematical techniques. There are physical examples, however, where disorder cannot be ignored, and chief among them are *spin glasses*. Indeed, the large body of literature on spin glasses appears to be motivated, at least in part, precisely because it presents a good example of a "disorderly system". Daniel L. Stein (1996) writes "From within the condensed matter physics community, spin glasses have come to present a problem that some feel to be among the deepest and most intractable facing us."

Rather than repeating descriptions from the literature, we ask you to please refer to the attached handout "Spin Glasses" (Stein (1989)) for a short introduction to the subject. Longer (but more difficult) treatments are given in Binder and Young (1986) and Mezard, Parisi, and Virasoro (1987).

This assignment will consider the use of linear programming (LP) methods to approach one of the fundamental spin glass problems, namely determining the *ground state* (the state of minimum energy). We will follow the ground-breaking method of Barahona and Maccioni (1982) in the assignment. The Barahona-Maccioni approach is developed further in Barahona, Grötschel, Jünger, and Reinelt (1988), Barahona (1994), and De Simone, Diehl, Jünger, Mutzel, Reinelt, and Rinaldi (1995). A web site containing some recent work in the area can be found at:

http://www.informatik.uni-koeln.de/ls_juenger/projects/spinglass.html

The model we consider consists of a finite set of *spins* $\mathcal{S}$ that take on values $+1$ or -1, corresponding to the magnetic orientation of the individual spins; this is called the "Ising model". There are prescribed levels of interaction for the spins, given by numbers J_{ij} for each pair of spins $S_i, S_j \in \mathcal{S}$, where the numbers depend on the impurities in the magnetic material and on the distance between the atoms (Barahona et al (1988)). Given a uniform external magnetic field of magnitude F (a number), the ground state energy can be computed via the optimization problem

$$\textit{minimize} \;\; H = \sum_{\{i,j\}} J_{ij} S_i S_j + F \sum_i S_i.$$

A common assumption is that only near-by spins S_i, S_j have non-zero interaction J_{ij}. To capture this near-by assumption, many studies represent the spins as points on a lattice, where spins only interact with the 4 adjacent lattice points (see Figure 1). To be able to

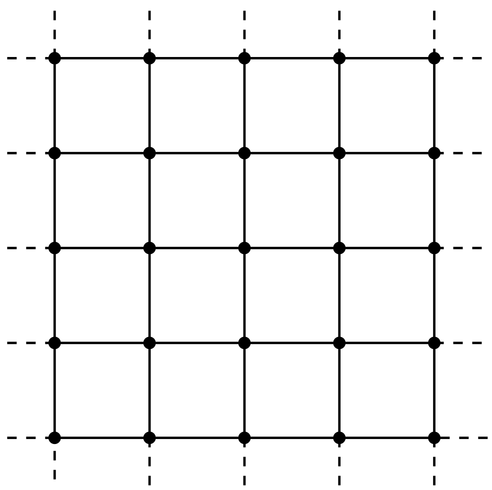

Figure 1: Lattice

work with a small finite model, researchers look at $n \times n$ grids of spins, where the spins on the border are joined to the spins on the opposite border (this can be viewed as a lattice on the torus); the graph for the 3×3 case is depicted in Figure 2. With this geometric view,

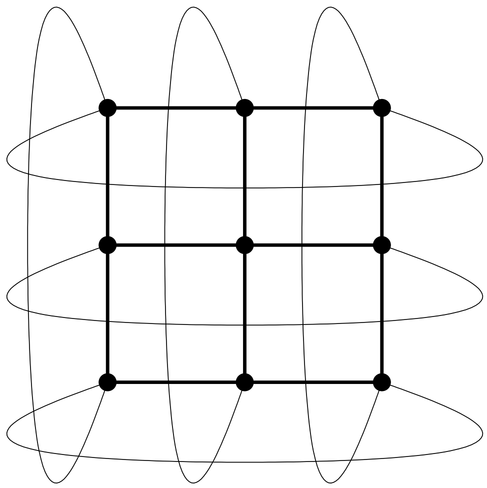

Figure 2: 3×3 toroidal grid

we can represent the magnetic field F as a extra node joined to every spin in the grid (see Figure 3).

In the physics literature, several types of interactions J_{ij} have been studied. We will focus on the Gaussian model, with the interactions chosen from a Gaussian (normal) distribution with mean $\mu = 0$ and variance $\sigma^2 = 1$.

Problem 1. Build a routine to generate random $n \times n$ Gaussian models, taking as input n

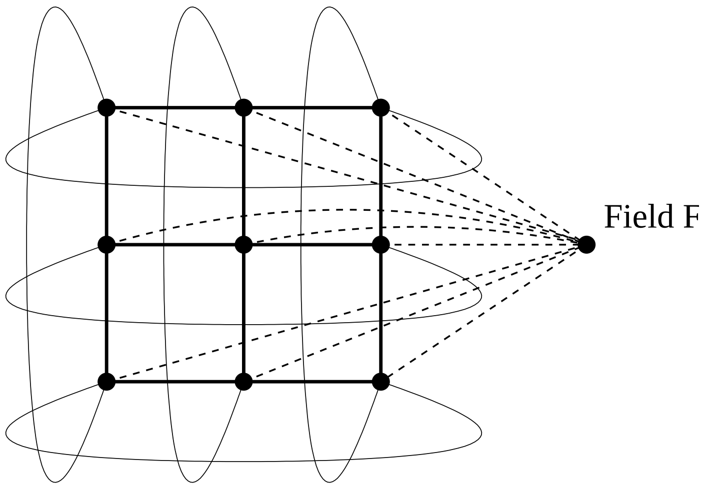

Figure 3: 3×3 grid with external field F

and the number F giving the level of the external field. The output of the routine should be a list of edges $e_{ij} = (i, j, w_{ij})$, where i and j are of type `int` representing nodes (either spins or the extra node for the external field; to make it easier to look at the model, please number the spins from 1 up to n^2, and use 0 to represent the extra node), and w_{ij} is of type `double` representing the weight of the interaction between the nodes (so $w_{ij} = J_{ij}$ if i and j are spins, and $w_{ij} = F$ if i is a spin and j is the extra node). Print a 3×3 example, with $F = 0.05012$. ▮

In most of the physics literature, heuristic algorithms (mainly simulated annealing) are used to estimate the ground state energy H for Ising models. This is a good way to obtain data for large examples, but it has the drawback that the estimates may not be accurate (and there is no easy way to know how far they differ from true values). Indeed, Barahona (1994) reports that differing estimates has led to some controversy in the spin glass community. The LP approach aims at obtaining exact values for H.

The output of the generation program (Problem 1) is an edge weighted graph $G = (V, E)$, where V is the set of nodes and E is the set of edges. An assignment of $+1$ or -1 to each of the spins corresponds to a partition of the node set V into two sets V^+ and V^- (we will assume that the extra node 0 is in V^+). The ground state energy for the assignment can be computed by examining the edges in the *cut* determined by V^+, that is, the set of edges joining nodes in V^+ to nodes in V^-. The cut is denoted by

$$\delta(V^+) = \{e_{ij} \in E : \ |\{i, j\} \cap V^+| = 1\}.$$

To see how to obtain H from the sum of the weights of the edges in $\delta(V^+)$, note that edges $e_{ij} \in \delta(V^+)$ contribute $-w_{ij}$ to H, edges e_{ij} with $i, j \in V^+$ contribute w_{ij} to H, and edges

e_{ij} with $i, j \in V^-$ also contribute w_{ij} to H (look at the original formula for H). So if we let

$$K = \sum_{e_{ij} \in E} w_{ij},$$

then

$$H = K - 2 \sum_{e_{ij} \in \delta(V^+)} w_{ij}.$$

Since K is a constant, we can minimize H by maximizing $\sum_{e_{ij} \in \delta(V^+)} w_{ij}$. This transformed problem is an instance of the *maximum-cut problem*, and we will use this transformation to determine H.

Problem 2. For the 3×3 example generated in Problem 1, obtain an estimate on the value of the maximum cut and use it to estimate H. (One way to compute the exact value of H is to solve the max-cut problem by checking all possible subsets of nodes, but there are 512 possibilities so you will want to let the computer check this for you.) ▮

The LP approach to spin glasses attempts to solve the max-cut problem via a "cutting-plane algorithm". For each edge $e \in E$ we have a variable x_e. If we have a set of nodes $Y \subset V$, then we identify the cut $\delta(Y)$ by setting $x_e = 1$ if $e \in \delta(Y)$ and $x_e = 0$ if $e \notin \delta(Y)$. Our goal is to set up an LP problem such that the optimum solution is a 0-1 vector that identifies the max-cut in the graph. Initially we choose as an LP

$$\begin{gathered} \text{Maximize } \sum(w_e x_e : e \in E) \\ \text{subject to} \\ 0 \leq x_e \leq 1, \text{ for all } e \in E. \end{gathered}$$

Problem 3. To start with a simple problem, use your LP platform (Ampl, Cplex, Excel, or some other program) to set-up and solve the above LP corresponding to your 3×3 test case. ▮

The solution of the initial LP should be a 0-1 vector, but it will not in general correspond to a cut in the graph (the optimal value DOES however produce an upper bound on the value of the maximum cut). We will try to coax the LP into producing a cut by selectively adding inequalities that are satisfied by every cut, but not satisfied by the optimal solution to the current LP. (This is the *cutting-plane method*, pioneered by Dantzig, Fulkerson, and Johnson.)

The additional inequalities we will add arise from cycles in the graph G. Note that if $C \subseteq E$ is a cycle, and $f \in C$ is an edge in the cycle, then any cut that contains f must also contain some other edge from C. This condition can be written as the inequality

$$x_f - \sum(x_e : e \in C \setminus \{f\}) \leq 0$$

that is satisfied by all cuts. More generally, if $F \subseteq C$ is a subset of edges and $|F|$ is odd, then every cut will satisfy the inequality

$$\sum(x_e : e \in F) - \sum(x_e : e \in C \setminus F) \leq |F| - 1.$$

We would like to use all of these *cycle inequalities* in our LP, but for large instances there will be far too many of them to write down (and to hope that our LP solver can deal with them). So we will only add in those that we need!

Problem 4. Starting with the initial LP solution, look for a cycle inequality that is violated by the solution, and add it to the LP formulation. Resolve the LP and repeat this procedure, until you (hopefully!) obtain a 0-1 vector that corresponds to a cut, and thus determine the exact ground state of the spin glass model. De Simone et al recommend that you first look for cycles corresponding to the squares in the toroidal grid, then look for cycles corresponding to the triangles formed with the extra node, then look for more general cycles. Note that it is possible that you end up with a solution vector x that is not 0-1 valued, but does satisfy all of the cycle inequalities. If this occurs, you have not solved the problem, but you do have a strong upper bound on the optimal value. ∎

Extra Credit

Problem X1. Try to automate the solution process by writing code that will search for cycle inequalities and add them to your LP. It is tough to search all cycles, but you can limit the search to the grid squares and to the extra-node triangles and still obtain good results. ∎

Problem X2. If you have a procedure where you do not have to do much work by hand, then try several other 3×3 or larger examples to see how the energy varies (keeping F fixed at the 0.05012 value). ∎

Problem X3. One way to handle the case where the cutting-plane method terminates with a solution that is not 0-1 valued is to add a branch-and-bound search based on the LP solution. This can be carried out by selecting an edge f such that x_f is fractional, and creating two sub-problems, setting $x_f = 0$ in the first sub-problem and $x_f = 1$ in the second sub-problem.

An alternative method is to give the final LP to an *integer* programming solver to (hopefully) produce an optimal 0-1 solution. If the 0-1 solution is a cut, then it gives the max-cut for the problem. If the 0-1 solution is not a cut, then you can add an additional inequality to the LP and again call the integer programming solver. This is much less work to implement (using, for example, Cplex's integer programming solver). ∎

References

F. Barahona (1994). "Ground-state magnetization of Ising spin glasses", *Physical Review B* **49**, 12,864–12,867.

F. Barahona and E. Maccioni (1982). “On the exact ground states of three-dimensional Ising spin glasses”, *Journal of Physics A, Mathematical and General* **15**, L611–L615.

F. Barahona, M. Grötschel, M. Jünger, and G. Reinelt (1988). “An application of combinatorial optimization to statistical physics and circuit layout design”, *Operations Research* **36**, 493–513.

K. Binder and A. P. Young (1986). “Spin Glasses: Experimental facts, theoretical concepts, and open questions”, *Reviews of Modern Physics* **58**, 801–963.

C. De Simone, M. Diehl, M. Jünger P. Mutzel, G. Reinelt, and G. Rinaldi (1995). “Exact ground states of Ising spin glasses: New experimental results with a branch and cut algorithm”, *Journal of Statistical Physics* **80**, 487–496.

M. Mezard, G. Parisi, and M. Virasoro (1987). *Spin Glass Theory and Beyond*, World Scientific Publishing Company, Singapore.

D. L. Stein (1989). “Spin Glasses”, *Scientific American*, July, 52–59.

D. L. Stein (1996). On the web at `http://www.physics.arizona.edu/physics/newsletter/winter96/spinglass.html`.