

Obtaining Ground States of Ising Spin Glasses via Optimizing Bonds Instead of Spins

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Ising spin glasses are prototypical models for disordered systems and have played a central role in statistical physics during the last three decades. In optimization, spin glasses provide a rich class of test problems that represent a challenge for most optimizers mainly because of the large number of local optima and the existence of rough energy landscapes. The primary purpose of this work is to describe a transformation of the problem of finding ground states of 2D and 3D Ising spin glasses in order to simplify the problem. More specifically, we propose a method to transform spin configurations into vectors of Boolean variables, one for each coupling constant ($S \rightarrow C$), and to transform the Boolean vectors for couplings back into spin configurations ($C \rightarrow S$). This enables an optimization algorithm to work in the space of coupling vectors instead of spin configurations. The effects of the proposed problem transformation are analyzed on a large number of 2D spin glass instances.

The proposed method is incorporated into the hierarchical Bayesian optimization algorithm (hBOA), the standard genetic algorithm (GA), and the univariate marginal distribution algorithm (UMDA). The problem transformation takes place after selection, creating a population of coupling vectors from the selected population of spin configurations. Essentially, the transformed problem contains one bit per coupling where the value of the bit specifies whether the corresponding coupling is satisfied or is unsatisfied in the spin configurations being transformed. After transforming the problem, variation operators are applied to coupling vectors, creating a new population of coupling vectors, which is subsequently transformed back into spin configurations. The new spin configurations are incorporated into the original population using restricted tournament replacement.

The tests were performed on 2D spin glasses of sizes 6×6 to 18×18 , 1000 random problem instances for each problem size. The results can be summarized as follows:

Effects on GA. For GA with two-point crossover, the proposed problem transformation leads to significant speedups that grow approximately linearly with problem size. For instances of 256 spins, this leads to speedups of 2 or more, depending on the settings.

Effects on UMDA. The speedups obtained with UMDA are much more dramatic than those obtained with the GA; already for the problem of size 100, the speedup of more than 720 has been obtained. Furthermore, while UMDA without the problem transformation was practically incapable of solving instances of 144 spins or more, UMDA with the transformed problem is easily able to solve even problems of 256 bits or more.

Effects on hBOA. Unlike GA and UMDA, hBOA does *not* benefit from the problem transformation at all; instead, we see that the problem transformation increases the number of function evaluations and the decrease in the performance gets more significant as problem size grows. We believe that the reason for this behavior is that hBOA is capable of discovering necessary problem regularities even without the problem transformation and the problem transformation thus leads only to the increase in the number of bits.

More details on this work can be found in Pelikan, M. & Hartmann, A. K. (2007), *Obtaining Ground States of Ising Spin Glasses via Optimizing Bonds Instead of Spins*, MEDAL Report No. 2007002, Missouri Estimation of Distribution Algorithms Laboratory, University of Missouri, St. Louis, MO. The report can be downloaded at <http://medal.cs.umsl.edu/files/2007002.pdf>

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