Letter

Equation Planting: A Tool for Benchmarking Ising Machines

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We introduce a method for generating benchmark problem sets for Ising machines—devices designed to solve discrete-optimization problems cast as Ising models. In our approach, linear systems of equations are cast as Ising cost functions. While linear systems are easily solvable, the corresponding optimization problems are known to exhibit some of the salient features of nondeterministic polynomial-time hardness, such as strong exponential scaling of heuristic solvers' runtimes and extensive distances between ground and low-lying excited states. We show how the proposed technique, which we refer to as "equation planting," can serve as a useful tool for evaluating the utility of Ising solvers functioning either as optimizers or as ground-state samplers. We further argue that equation-planted problems can be used to probe the mechanisms underlying the operation of Ising machines.

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I. INTRODUCTION

In recent years we have witnessed a flourishing of experimental "Ising machines"—special-purpose programmable devices engineered to solve discrete-optimization problems [1,2] cast as Ising models—with the tacit promise that their performance is superior to that of algorithms running on standard computers. Analog quantum devices that perform quantum annealing [3,4] designed to find bit assignments that minimize the cost of Ising Hamiltonians have already been realized on various platforms, such as arrays of superconducting flux qubits [5–11]. Other notable technologies that recently emerged are coherent Ising machines based on lasers and degenerate optical parametric oscillators [12,13], quantum-inspired digital annealers based on field-programmable gate arrays [14], and memcomputing devices that operate on terminal-agnostic self-organizing logic gates [15–17].

With improved performance over traditional algorithms [18,19], Ising machines have gained a large amount of interest, both in the academe and among the general public—and rightfully so. Many problems of theoretical and practical relevance, in areas as diverse as machine learning, materials design, software verification, portfolio management, and logistics, can be cast as searching for the global minima of Ising cost functions [1,2]. It is, however, unclear to date whether any one of the aforementioned devices truly offers genuine advantages over its competitors.

One of the main bottlenecks preventing meaningful benchmarking of Ising machines is the absence of appropriate benchmark problems. Generating problem instances that are, on the one hand, challenging enough and whose solutions are, on the other hand, known in advance or are easily verifiable, so as to allow proper benchmarking, is not straightforward since these two requirements are, in many respects, contradictory. To overcome this obstacle, various methods have been devised in recent years to generate problem classes with known minimizing configurations (see, e.g., Refs. [20–22]). However these have generally been found to lack the hardness that characterizes problems that are nondeterministic polynomial-time (NP) hard. At the other extreme, problem classes that are challenging to solve but whose ground-state energies are not verifiable have also been developed [23–25].

To bridge the aforementioned gap, in this study we present a method for generating benchmark problem sets for Ising machines that we argue may serve as a suitable tool for evaluating their performance and in turn also to indirectly probe the mechanisms underlying their operation. The proposed technique, which we refer to as "equation planting," has several desirable properties. Explicitly, the problem sets generated, while generated from easily solvable problems, possess some of the salient features of NP-hard problems—most notably extensive distances between ground and low-lying excited states.

Our approach is based on the embedding of linear systems of equations in Ising models, motivated by the observation that when linear systems of equations are cast as optimization problems, the latter form often stymies heuristic solvers [26–31]. In addition to presenting a method for generating benchmark problem sets for Ising machines functioning as optimizers, we also show that the

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proposed technique may be used to test the functionality of these devices as Boltzmann samplers, or more specifically as ground-state samplers [32–34], because of another property of these problem sets—namely, a verifiable number of ground-state configurations.

We begin by describing the equation-planting technique in general, moving on to focus on a specific class of problem instances, which we use to demonstrate the effectiveness of the method.

II. EQUATION PLANTING

We begin by considering a linear system of m equations in n variables:

$$\sum_{j=1}^{n} a_{ij} x_j = b_i \quad \text{for } i = 1 \ldots m, \tag{1}$$

where $\{x_1, \ldots, x_n\}$ stand for variables over a given field, and $\{a_{ij}\}$ and $\{b_i\}$ are the equation coefficients. Every such linear system may be cast as an optimization problem with the corresponding cost function

$$F = \sum_{i=1}^{m} \left\| \sum_{j=1}^{n} a_{ij} x_j - b_i \right\|^2 . \tag{2}$$

Since F is a sum over positive terms, any configuration $\{x_1^*, \ldots, x_n^*\}$ that yields $F = 0$ is a minimizing configuration that also solves the linear system.

As already mentioned, even though the computational problem of solving a linear system of equations is easy—any given instance can always be solved in polynomial time using Gaussian elimination—the corresponding optimization problem is not necessarily easy for heuristic solvers [26,27,29–31].

We leverage the above setup toward constructing Ising problems that stymie heuristic solvers. To that aim, we focus henceforth on linear systems of equations modulo 2; that is,

$$\sum_{j=1}^{n} a_{ij} x_j = b_i \mod 2 \quad \text{for } i = 1 \ldots m, \tag{3}$$

where now both the variable set and the coefficients are Booleans taking on values $\{0, 1\}$. The ith equation can therefore be written as $\bigoplus_{j:a_{ij}=1} x_j = b_i$ (here $\oplus$ denotes the bitwise XOR operation), or in terms of Ising spins $s_i \in \{-1, 1\}$,

$$\prod_{j:a_{ij}=1} s_j = (-1)^{b_i}. \tag{4}$$

Cast in optimization form, the system of equations becomes

$$\tilde{F}_2 = \sum_{i=1}^{m} \left(\prod_{j:a_{ij}=1} s_j - (-1)^{b_i} \right)^2 , \tag{5}$$

or, after immaterial constants have been dropped,

$$F_2 = -\sum_{i=1}^{m} (-1)^{b_i} \prod_{j:a_{ij}=1} s_j . \tag{6}$$

The cost function F_2 is a multispin cost function consisting of a sum of products of spin variables. The localities of the terms composing the cost function are precisely the number of variables in the corresponding equations. The minima of F_2 correspond to the solutions of the system given in Eq. (4), provided that solutions exist. In more detail, linear systems may behave in one of three possible ways: (i) The system may have no solutions at all. This scenario corresponds to the cost function $\tilde{F}_2$ having a strictly positive minimal value (meaning $F_2 > -m$) and may happen if the number of equations is greater than the number of variables. (ii) The system may have a unique solution. Here a single configuration minimizes F_2, whose minimal value in this case would be $-m$. (iii) The system may have multiple solutions if the dimension of its null space, or nullity [35], which we denote here by d_N, is nonzero. In this case, the number of minimizing configurations that yield $F_2 = -m$ is $N_{\text{sol}} = 2^{d_N}$.

Ising machines are designed to tackle two-body cost functions. The locality of the multispin cost function F_2 in this case may be readily reduced to a two-body Ising model of the general form $\sum_{ij} J_{ij} s_i s_j + \sum_i h_i s_i$ using standard reduction techniques (see, e.g., Ref. [36]), where $\{J_{ij}\}$ and $\{h_i\}$ are integer-valued coefficients.

As we demonstrate in the next section, while the solutions of the linear systems of equations used to generate these Ising cost functions are straightforwardly obtained (if there are any), heuristic solvers will generically find problems of this type extremely difficult to solve. In what follows, we illustrate this by studying in detail one specific type of equation system—namely, the random 3-regular 3-XORSAT (3R3X) system, where XORSAT stands for "exclusive or satisfiability".

III. 3-REGULAR 3-XORSAT SYSTEM AS A TWO-BODY ISING MODEL

To demonstrate the challenges that equation-planted instances present to heuristic Ising solvers, we consider as a test case linear systems modulo 2 (also known as "XORSAT equations") wherein each equation contains exactly three randomly chosen Boolean variables and each variable, or bit, x_j appears in exactly three equations.

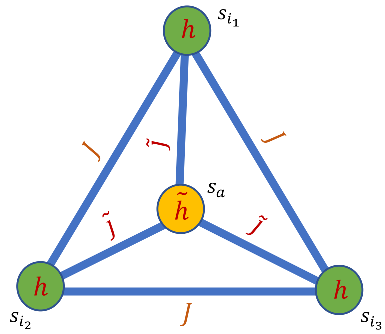

FIG. 1. The two-body 3-XORSAT gadget. The gadget is a fully connected spin quadruplet with parameter values $(h, \tilde{h}, J, \tilde{J})$ as described in the main text. The four minimizing configurations of the 3-XORSAT clause are encoded in the ground states of the Ising cost function of the gadget restricted to spins $s_{i_1}, s_{i_2}, s_{i_3}$. The spin s_a serves as an auxiliary spin.

This type of problem is also known as a "3-regular 3-XORSAT problem" and was studied in various contexts [28,30,31,37,38]. An n-bit instance would thus consist of n equations of the form $x_{i_1} \oplus x_{i_2} \oplus x_{i_3} = b_i$ [39]. While the results presented below pertain to the 3R3X system, they should extend in general to other classes of linear XORSAT systems.

The cost function F_2 of an n-bit 3R3X system is therefore the sum of n three-body terms of the form $-(-1)^{b_i} s_{i_1} s_{i_2} s_{i_3}$ defined on n Ising spins. To reduce the locality of a term to two-local and one-local terms, we use a gadget that shares its four minimizing configurations [39]. For the negatively signed clause ($b_i = 0$), these are the four configurations whose product is positive, namely, $(1, 1, 1)$, $(1, -1, -1)$, $(-1, 1, -1)$, and $(-1, -1, 1)$, and an appropriate gadget is

$$G_{3X} = h(s_{i_1} + s_{i_2} + s_{i_3}) + \tilde{h} s_a + J(s_{i_1} s_{i_2} + s_{i_2} s_{i_3} + s_{i_3} s_{i_1}) + \tilde{J} s_a (s_{i_1} + s_{i_2} + s_{i_3}), \quad (7)$$

where $(h, \tilde{h}, J, \tilde{J})$ can be either $(-1, -2, 1, 2)$ or $(-1, 2, 1, -2)$, yielding in both cases a minimal cost of -4 (other gadgets exist that can equivalently be used). The above gadget is a fully connected four-spin cost function with s_a serving as an auxiliary spin (see Fig. 1). The positively signed clauses are treated similarly.

The gadget allows us to cast n-bit 3R3X linear systems as two-body Ising models with $2n$ spins, as each clause adds one auxiliary spin to the problem and an n-bit instance has n clauses.

At this point, we note several of the properties of 3R3X Ising instances: (i) These instances have a bounded degree (namely, 9) as each spin connects in general to three other spins for every clause in which the spin appears. (ii) The specification of Ising parameters $\{J_{ij}\}$ and $\{h_i\}$ requires only two bits of precision as both spin-spin couplings and longitudinal fields are integers in the range $[-3, 3]$. (iii) As already mentioned, these instances have known ground-state energies. (iv) These instances have a controllable ground-state degeneracy, determined by the nullity of the generating linear system. As will become evident in the next section, these properties may be leveraged to determine the utility of heuristic Ising solvers functioning either as optimizers or as ground-state samplers.

IV. RESULTS

In what follows, we examine the performance of heuristic solvers on randomly generated two-body 3R3X Ising instances that have unique solutions. As a representative of state-of-the-art heuristic solvers, we use parallel tempering (PT) [40,41]—a refinement of the celebrated yet somewhat-outdated simulated-annealing algorithm [42], which finds the ground-state configurations of general discrete-variable cost functions [20,24,37,43–49]. In PT,

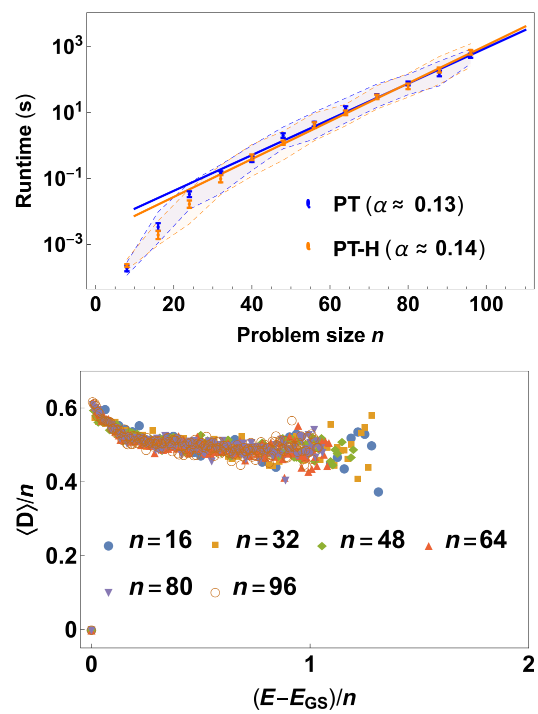

FIG. 2. Runtime scaling of two parallel tempering variants on random 3R3X-planted Ising instances on a log-linear scale (top). Typical runtimes (median over 100 instances) as a function of problem size are given for PT and PT-H. Both exhibit similarly strong exponential scaling. Fits to $e^{\alpha n}$ are shown. Error bars correspond to 1σ statistical confidence. The shaded areas correspond to the interquartile ranges for each problem size. Typical Hamming distances $\langle D \rangle$ (normalized by problem size) of local minima from the global minimum as a function of normalized residual energy are also shown (bottom). The plot demonstrates that low-lying excited states are typically $O(n)$ spin flips away from the global minimum.

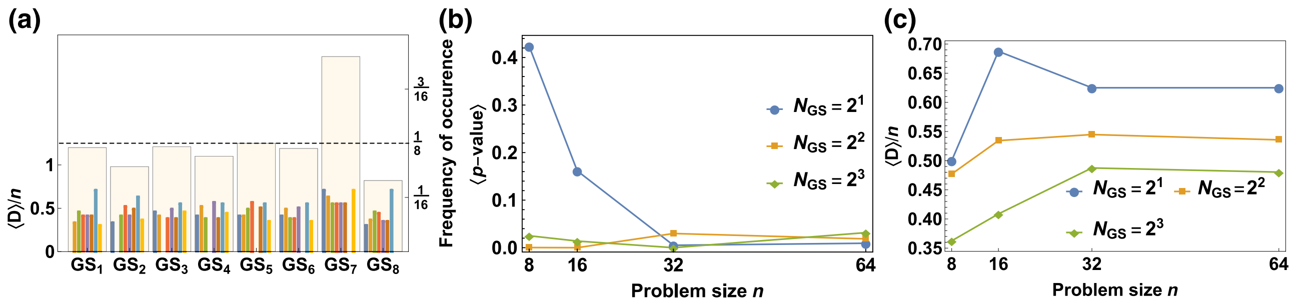

FIG. 3. Fraction of ground-state occurrences for a random 64-spin 3R3X instance with an eightfold ground-state degeneracy as found by 1000 parallel tempering runs (left). The horizontal dashed line corresponds to uniform sampling. Also shown are the normalized Hamming distances $\langle D\rangle$ between each ground state and all other states. Typical p values obtained from a one-sided χ^2 test performed on the ground-state occurrences of randomly generated instances with twofold, fourfold, and eightfold ground-state degeneracies as a function of problem size n (middle). Typical normalized Hamming distances between the ground states of degenerate instances as a function of problem size n for different nullities (right).

multiple copies of the problem are equilibrated in parallel at different temperatures and spin configurations at adjacent temperatures are regularly swapped [39]. In addition, we consider a variant of PT (which we denote as "PT-H") that uses global cluster moves due to Houdayer [50] and is known to accelerate PT convergence rates for many problem classes (see, e.g., Refs. [51–53]).

We test the performance of PT and PT-H on instances of various sizes by measuring their typical times to find minimizing configurations. Here typical runtimes are defined as the median time to reach a minimizing configuration over 100 randomly generated instances of a given size [54].

The results are presented in the top part of Fig. 2, which shows the exponential runtime scaling of both PT and PT-H with problem size, proportional to $e^{\alpha n}$, with $\alpha \approx 0.13$ and $\alpha \approx 0.14$, respectively, indicating a strong exponential scaling. Moreover, the Houdayer cluster updates do not seem to improve the scaling. Also shown in the top part of Fig. 2 (as shaded areas) are the interquartile ranges (the difference between the 75th and 25th percentiles) of the PT and PT-H runtimes, quantitatively indicating the homogeneity in the hardness of the instances.

To better understand why these problems, while being trivial to solve using Gaussian elimination, present severe challenges to heuristic solvers, we next examine their energy landscapes. We do so by measuring the Hamming distances between local-minimum configurations, as found by the solver in the course of the simulation, and the global minimum. These are plotted in the bottom part of Fig. 2. The low-lying excited states, characterized by small yet positive residual energies, are typically approximately $0.6n$ spin flips away from the global minimum, implying that reaching a local minimum is not an indication of the whereabouts of the ground state. The above property is a hallmark of NP-hard problems [2].

We next illustrate the usefulness of equation planting in determining the bias of Ising machines tasked with sampling the ground-state manifolds of Ising cost functions [24,55,56], which in addition to optimization is considered to be one of their main suggested uses [32–34,49].

We first construct random Ising-encoded 3R3X instances with nullities $d_N = 1, 2, 3$ having ground-state degeneracies of 2, 4, and 8, respectively, at different problem sizes. We then study the functionality of PT-H as a ground-state sampler by simply measuring the fraction of occurrences of each ground state for any given instance (see Fig. 3, left plot). Each instance is solved 100 times, and the ground-state configurations are recorded.

We quantify the bias of PT-H on the various instances by measuring the typical p value obtained from one-sided χ^2 tests performed on the tallied ground states of each instance under the hypothesis that the true distribution is uniform. The results are summarized in the middle plot in Fig. 3. The smallness of the p values indicates PT's strong bias in sampling ground-state manifolds of these instances, implying differently sized "basins of attraction" for each ground state. We also find that, similarly to the ground state manifolds of NP-hard problems, the distances between the ground states of any given instance are typically extensive. These are depicted in the right plot in Fig. 3 [57].

V. SUMMARY AND CONCLUSIONS

We introduce a method for generating random problem sets that we argue are optimally suitable for verifiably testing the utility of Ising machines. The proposed technique allows the construction of random problem sets that have a number of properties that are desirable for this task: (i) verified ground-state energies; (ii) controllable ground-state degeneracy; (iii) "NP-hard-like" energy landscapes; (iv) low-precision problem parameters; and (v) underlying connectivity with a bounded degree.

We further illustrate the computational difficulties that heuristic state-of-the-art solvers face when tasked with finding or uniformly sampling the minimizing configurations of problem sets possessing intricate energy landscapes. We show that equation-planted instances are difficult to solve even at small sizes, revealing rather early on the asymptotic exponential scaling expected from heuristic solvers. In addition, we note that, as is expected from difficult problem sets, Houdayer cluster moves [50] do not provide any additional advantages.

With the above stated, it should be noted that since the problem sets are generated from trivially solvable systems, special-purpose algorithms could conceivably be tailored to identify the underlying equations within the Ising cost function and utilize the equation structure to solve these Ising cost functions polynomially fast. On the other hand, the equation structure can be easily obfuscated if one (i) uses a wider range of gadgets to embed the various XORSAT clauses, (ii) constructs instances using a randomly weighted sum of terms, (iii) generates nonregular linear systems of equations with potentially different numbers of variables per equation, or (iv) adds to existing XORSAT cost functions non-XORSAT gadgets whose ground states coincide with those of the instance, as these are known in advance. An interesting question that arises in this context is whether one can obfuscate such easily solvable problems in a manner that is provably intractable to "reverse engineer" to an easily solvable form.

In the generation of the random XORSAT instances considered in this study, no specific connectivity constraints are assumed, which in turn leads to the generation of Ising instances with random connections among the various spins. These instances could not be directly programmed into Ising machines that have rigid and sparse architectures [34]. This limitation may be addressed in one of two ways. The first is to convert the randomly connected instances to match the Ising-machine hardware graph via embedding schemes at the price of adding auxiliary spins to the problem [58]. Alternatively, one can directly generate equation-planted instances that are native to the device connectivity, which may require novel 3-XORSAT gadgets to be devised.

Another aspect of equation planting that has not been explored here is the relative hardness of r-regular k-XORSAT instances for different k, r greater than 3—problem classes that are expected to yield yet-harder instances. Varying k, r would presumably allow "hardness tunability," which is often a desired property in the benchmarking of heuristic solvers. Another way of achieving hardness tunability that was not pursued here is the use of nonregular random graphs, such as Poisson graphs, rather than random regular graphs [27].

The NP-hard-like energy landscapes characterizing equation-planted instances coupled with the fact that their ground-state manifolds can be known in advance may also be used as a tool for gaining insight into the mechanisms underlying the operation of Ising machines. This is because the machines' performance on these problems serves as an indicator of the locality of the heuristic being use. As we demonstrated above, local search approaches are not very successful, whereas global approaches such as Gaussian elimination are able to decipher their inherent structure very easily. Another possible use of problems of this type is the study of spin glasses, specifically the onset of temperature chaos [43,59,60].

One intriguing future research direction would be the development of heuristic solvers that identify XORSAT-type relations between the spins of Ising cost functions and utilize the ease with which such subproblems can be minimized so as to efficiently find global minimal costs.

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