LOW AUTO-CORRELATION BINARY SEQUENCES EXPLORED USING WARNING PROPAGATION

"WARNING PROPAGATION" PARA SECUENCIAS BINARIAS DE BAJA AUTOCORRELACIÓN

O. E. Martínez-Durive[a†], I. Kotsireas[b], R. Mulet[a], A. Lage-Castellanos[a]

a) Group of Complex Systems and Statistical Physics, Physics Faculty, University of Havana, Cuba[†]
b) Wilfrid Laurier University, Waterloo, Canada
† corresponding author

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The search for binary sequences with low auto-correlations (LABS) is a computationally hard discrete combinatorial optimization problem. We analyze two physically inspired algorithms to explore the low energy space of this model. The greedy, $T = 0$, Monte Carlo (MC) method gets trapped into the exponentially many 1-Spin-Flip stable configurations, that are typically low in energy, but still far from the global optimum. The more elaborated Warning Propagation (WP) algorithm also gets trapped into local minima. However, these local minima, are more stable to spin flips than the ones obtained by the greedy MC. We also compare the behavior of both algorithms in randomized versions of LABS, showing that the low energy space of the 4-Spin model is easier to explore than the one of LABS.

La búsqueda de Secuencias Binarias de Baja Autocorrelación (LABS) es un problema de optimización combinatoria difícil. Analizamos dos algoritmos inspirados en la física para explorar el espacio de bajas energías de este modelo. El algoritmo de Monte Carlos (MC) a $T = 0$ queda atrapado entre la cantidad exponencial de estados semi-estables que se encuentran en la región de bajas energías pero lejos del mínimo global. El algoritmo de Warning propagation (WP), más elaborado que MC, también queda atrapado en esta región. No obstante los estados de baja energía que se obtienen con WP son más estables que los obtenidos por MC. Además comparamos el comportamiento de ambos algoritmos en versiones aleatorizadas de este modelo, mostrando que la región de baja energía del 4-Spin es más fácil de explorar que en LABS.

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I. INTRODUCTION

The Low Auto-correlation Binary Sequence (LABS) problem consists in finding a binary sequence $S = \{S_1, S_2, ..., S_N\}$ where $S_i \in \{1, -1\}$ for $1 \leq i \leq N$ that minimizes the function

$$E(S) = \sum_{k=1}^{N-1} C_k(S)^2 \tag{1}$$

where $C_k(S)$ are the aperiodic auto-correlation coefficients

$$C_k(S) = \sum_{i=1}^{N-k} S_i S_{i+k}. \tag{2}$$

Finding the optimal sequences is notoriously hard for increasing values of N [1].

These low auto-correlation binary sequences have many practical applications (see comments in [2]) like signal processing [3, 4], Artificial Intelligence [5], and is connected to the Littewood problem in Mathematics [6].

The problem has been largely studied using exact and heuristic methods. The exhaustive search has a time complexity of $O(2^N)$ and was used [7] to find optimal sequences up to $N = 32$. Other works applied a Branch and Bound algorithm, which is an exact method, reducing the computational cost to $O(c^N)$ with $c < 2$. On [8] the value of c was taken to $c = 1.85$, exploring sequence up to $N = 48$. Later, on [9] it was proposed a new bound function with a lower $c = 1.8$. On 2010, a more tight bound was proposed [10] and the algoritmh was deployed on a GPU cluster, finding the optimal sequences up to $N \leq 64$ with $c = 1.79$. Finally, on 2016, using a combination of the last two bounds in [2], and with a estimate value of $c = 1.729$ it was possible to find the best know sequences up to $N \leq 66$. Despite these sophisticated implementations and improvements it is clear that this approach is not viable in the search of optimal sequences with larger lengths, say $N > 100$, for instance.

Heuristic methods have also been largely studied, as the evolutionary search [11], memetic algorithms [12] and tabu search [13, 14] reaching sizes $N \in [61 - 77]$ with a computational cost of $O(1.34^N)$. A readable summary of the application of different heuristic and stochastic algorithms to LABS appears in [5] and [1]. The state of the art of heuristic algorithms according to [2] seems to be the work [1] where the authors combined a random self-avoiding walk in a Hasse graph. However, as in the case of exact algorithms, these complex and advanced heuristics fail in systems of relative big sizes ($N > 200$) [2] leaving a lot of room for further improvements.

In Statistical Physics, the low autocorrelation sequences can be seen as the ground states of the Bernasconi's model [15], that implies the energy minimization of an Ising spin system with long range interacting variables with four-fold antiferromagnetic interactions.

This paper characterizes two well known simple physical

inspired algorithms on LABS instances. First, Greedy Monte Carlo (MC) and Warning Propagation (WP) are introduce and compared showing that indeed, WP it is a better candidate to look for low energy configurations of the LABS problem. Later, WP is tested on disordered versions of LABS to shed light on the structure relevance of the underlying graph.

II. PHYSICALLY INSPIRED ALGORITHMS

The minimization of the energy $E(S)$ (cost function) can be obtained by specific methods tailored for this very problem, as those that are the state of the art for LABS, or conversely by general standard techniques. While the former are currently more efficient the later are easier to interpret and may open the way to new disruptive ideas in the treatment of the problem. The simplest of these algorithms is the greedy minimization of the cost function. A simple greedy approach corresponds in the statistical mechanics community to the Monte Carlo method at $T = 0$, where variables are iteratively altered only when the proposed changes reduce the energy. It can also be seen as a discrete-variable version of a steepest descent optimization method. Typically greedy algorithms are simple to program and guaranteed to converge, but are prone to lock on non-optimal solutions.

On the other hand, since the beginning of the century, Message Passing algorithms have found their way in the realm of the statistical physics community. The turning point was the realization that message passing algorithms can be viewed as fixed point equations derived from variational approximations to the free energy of Ising-like models [16]. This inspired researchers to look for novel applications of these algorithms in the field of Combinatorial Optimization [17–19] and to explore new extensions [20–22].

In statistical physics the cost function is alternatively interpreted as the Hamiltonian or the Energy of the model. In the case of LABS (1) it can be represented by a standard factor graph [16], where both the variables and their interactions are graphically represented. Let take as an example the part $C_{k=1}(S)^2$ of the LABS hamiltonian (1) with $N = 5$ spins

$$\begin{aligned} C_{k=1}(S)^2 &= \left(\sum_{i=1}^{5-1} S_i S_{i+1}\right)^2 \\ &= (S_1S_2 + S_2S_3 + S_3S_4 + S_4S_5)^2 \\ &= \text{const} + 2(S_1S_3 + S_2S_4 + S_3S_5 + \\ &\quad S_1S_2S_3S_4 + S_1S_2S_4S_5 + S_2S_3S_4S_5). \end{aligned} \tag{3}$$

Since $S_i = \pm 1$ are binary, every square value $S_i^2 = 1$ can be disregarded as constant. Intuitively, the goal is to find a configuration of the variables that produces as many negative summands as possible. Each summand coorresponds to an interaction, represented in the factor graph as a square node (see Fig. 1), while the variables interacting are represented as circles, joined to their corresponding interactions by an edge in the factor graph. Factor nodes index will be referred using a, b, c letters, and i, j, k for refer to the variables index. The notation $N(a)$ will be used to refer the set of variables that interact with the factor node a, and similar $N(i)$ for the set of factor nodes that interact with variable i.

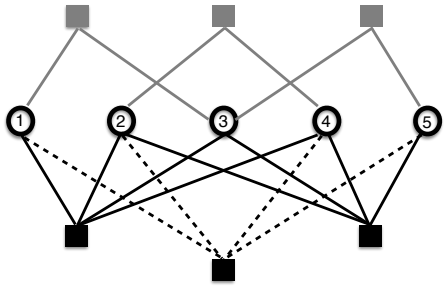

Figure 1. Graphical representation of equation (3). The variables (circles) are connected to interactions (square nodes). In gray, the three first terms (connecting only two variables), in black the other three 4-spins interactions.

II.1. *Greedy minimization: Monte Carlo at $T = 0$*

The condition for a given configuration $\{S_1, S_2, \ldots, S_N\}$ to be a local energy minimum of LABS can be written in the following way

$$S_i = \text{sign}(H_i) \tag{4}$$

$$\text{where} \quad H_i = \sum_{b \in N(i)} U_{b \to i}$$

$$\text{and} \quad U_{a \to i} = -\text{sign}(S_j S_l S_k). \tag{5}$$

In this notation, $U_{a \to i}$ acts as the local opinion of the interaction a on which direction should the variable S_i be pointing to, while $S_i = \text{sign}(H_i)$ ensures that each variable points to the direction suggested by the majority of its factor nodes. A local minimum is the situation in which every spin points in the direction of its total field. Configurations satisfying such condition can not minimize its energy with a unique spin-flip, and therefore are called 1-spin flip stable configurations (1-SFS).

The greedy Monte Carlo algorithm corresponds to the sequential search for 1-SFS states by randomly modifying the variables that are frustrated $S_i H_i < 0$, as shown in Algorithm

Require: Set of spins $\{S_1, \ldots, S_N\}$, and a set of interactions $\{a = (S_i, S_j, S_k, S_l), b = (S_h, \ldots), \ldots\}$.
Ensure: Returns 1-spin flip stable configuration
  $\vec{S}$ = Random-Select($\{\pm 1\}^N$) {Take a random starting sequence}
  Compute all messages $U_{a \to i}$ and H_i using eq. (5)
  $F_{set} = \{i | S_i H_i < 0\}$
  while F_{set} not empty **do**
    j = Random-Select(F_{set})
    $S_j = -S_j$ {Flip a frustrated spin}
    Compute all messages $U_{a \to i}$ and H_i using eq. (5) {Actually only those affected by the flip}
    $F_{set} = \{i | S_i H_i < 0\}$
  end while
  return $\vec{S}$

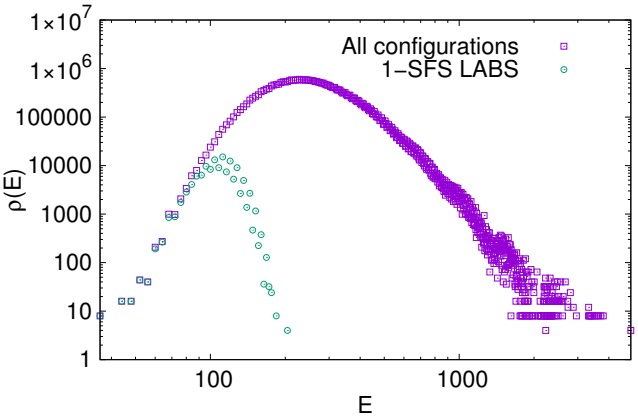

Figure 2. Density of states and density of 1-Spin flip stable configurations for the LABS problem with $N = 25$. Both results obtained from an exhaustive enumeration of all the 2^{25} configurations.

It is easy to show that at every iteration, the total energy of the system is reduced. Since such energy is bounded by below greedy Monte Carlo has the following properties

1. the algorithm stops after a finite number of steps
2. the state found is a 1-SFS configuration, meaning that the total energy of the system can not be lowered by a single spin change.

Of course, the binary sequence with the lowest autocorrelation is one of such 1-SFS states, since it is the absolute energy minimum. However, there are (exponentially in N) many such stable states (see Fig. 2), and Monte Carlo greedy minimization will usually get stuck in one of them, far from the global optimum.

II.2. Warning Propagation

Message passing algorithms, like sum-product [23], belief propagation [16], and warning propagation [24] have been derived more than once in different communities and for different applications, with different balances between rigor and intuition. A standard approach presents them as an approximation to study the properties of the measure

$$P(S) = \frac{1}{Z} \exp\left(-\beta E(S)\right). \tag{6}$$

In the limit of low temperatures ($\beta = 1/T \to \infty$) the measure concentrates on the configurations of lowest energy, and therefore good approximations can be transformed into good optimization procedures. Warning propagation corresponds to the zero temperature limit of the Bethe approximation in statistical mechanics. Said in other terms, the max-sum algorithm corresponds to the zero termperature limit of the sum-product one (standard belief propagation).

WP is implemented in terms of two types of messages: $U_{a\to i}$ carrying information from interaction node a to any of its variables i, and the converse $H_{i\to a}$ sending information from variable i to one of its interactions. It is possible to derive the following two equations relating these messages by taking the appropriate $T = 0$ limit in the belief propagation equations

$$\begin{aligned} U_{a\to i} &= -\operatorname{sign}\left(H_{j\to a} H_{l\to a} H_{k\to a}\right) \\ &= -\operatorname{sign}\left(\prod_{j\in N(a)\setminus i} H_{j\to a}\right) \end{aligned} \tag{7}$$

$$H_{i\to a} = \sum_{b\in N(i)\setminus a} U_{b\to i}. \tag{8}$$

The expresion $U_{a\to i}$ is expanded for the case of factor nodes a with four variables, but it is clear from the compacted form that in the case of two-variables factors, the equation reduces to $U_{a\to i} = -\operatorname{sign}(H_{j\to a})$.

The WP equations are a "cavity" version of the Monte Carlo ones (5), where the cavity term refers to the fact that self interaction $U_{a\to i}$ is removed from (8) in the definition of the field $H_{i\to a}$.

The Warning Propagation algorithm consists of iterating the messages eqs. (7, 8) until convergence, as shown in algorithm:

Require: Set of interactions $\{a = (S_i, S_j, S_k, S_l), b = (S_h, \ldots), \ldots\}$, maximum number of iterations T_{max}.
Ensure: Returns a fixed point of WP, or "NonConverged".
  Initialize all fields $H_{i\to a}$ picking uniform from {-1, 0, 1}.
  while $T < T_{max}$ and NotConverged **do**
    NotConverged = False
    Order = Random-Shuffle([1:N])
    for (i in Order) **do**
      for $a \in N(i)$ **do**
        Update $U_{a\to i}$ y $H_{i\to a}$ as in eq. (7) and (8)
        if $U_{a\to i}$ or $H_{i\to a}$ changed **then**
          NotConverged =True
        end if
      end for
    end for
  end while
  if $T < T_{max}$ **then**
    Compute total fields $H_i = \sum_{b\in N(i)} U_{b\to i}$
    return $\vec{S} = (\operatorname{sign} H_1, \operatorname{sign} H_2, \ldots, \operatorname{sign} H_N)$
  else
    return "Non Converged"
  end if

There is a trivial fixed point of this algorithm, where all messages are zero, but it is highly unstable, and even a tiny fraction of non zero messages at the beginning takes the algorithm to other non-trivial and more informative fixed points. In the case that the algorithm reaches convergence (fixed point of the fields), you can recover a local energy minimum by setting the total field to $H_i = \sum_{b\in N(i)} U_{b\to i}$ and the spins to $S_i = \operatorname{sign} H_i$. We found that WP generally converge in instances of LABS, however, it requires running times that are orders of magnitude larger than Monte Carlo. This disadvantage is partially compensated by a nice property:

1. fixed point solutions of warning propagation correspond to configurations that are stable with respect

to flipping any set of interacting variables that are singly connected (a tree), or belong to a single loop, or to a disjoint union of these types of sets [25].

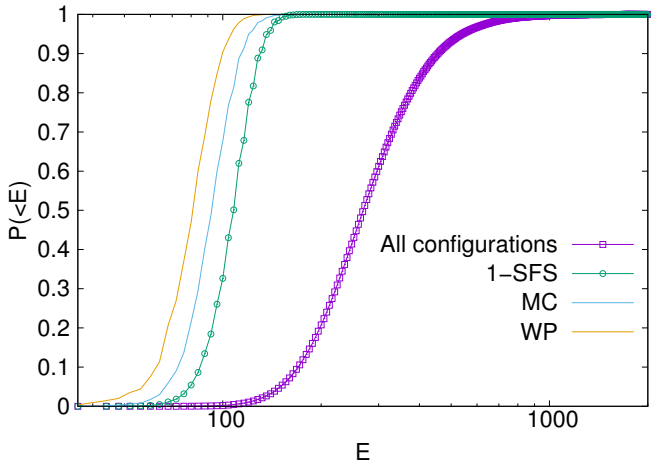

Figure 3. Cummulative distribution of energies for MC T=0 and WP compared to the density of 1 Spin-flip stable configurations for LABS $N = 25$. WP explores the lower energies more frequently than MC, and both explore the very low energy sub-space of the configurations space.

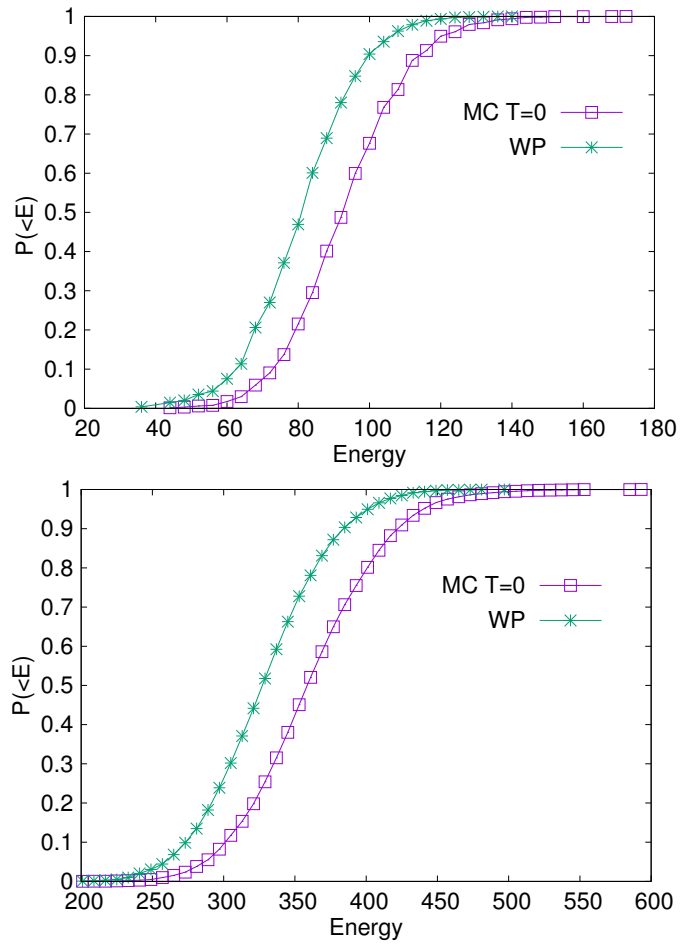

Figure 4. Top, $N = 25$, bottom $N = 50$. Cummulative probability of finding configurations below a given energy for Greedy Monte Carlo and Warning Propagation. In both figures Warning Propagation algorithm is shown to outperform Greedy Monte Carlo.

This implies that all WP fixed points are also Monte Carlo stable states, while the reverse is not true. The number of fixed points of WP is usually also large, but being the stability requirement more demanding, they are expected to be fewer and concentrate at lower energies than those of $T = 0$ Monte Carlo. For this reason, WP seems a good candidate to attack the optimization in LABS.

Figures 3 and 4 show the distribution of energies for the states given by both algorithms Greedy Monte Carlo at $T = 0$ and Warning Propagation. Figure 3 points to the fact that both MC and WP concentrate in the very low part of the full spectrum of energies for a small system $N = 25$. Fig 4 zooms into the low energies and shows the cumulative probability function of the energies of the resulting states after 1000 runs of Monte Carlo and WP for two system system sizes $N = 25, 50$. As expected, Warning Propagation finds low energy configurations with higher probability. However, neither of the algorithms is particularly good at finding the global optimal configurations at $E^0_{25} = 36$ and $E^0_{50} = 153$ respectively.

Finally, Fig. 5 shows the average behavior of both algorithms at growing values of N. Both algorithms find typical states (see symbols for Mean MC, Mean WP) with an energy that is much lower than the typical energy of a LABS sequence at random (Mean LABS), indeed far more lower than one standard deviation of the energy spectrum. This mean that they found rare configurations of low energy. Moreover, Warning propagation is always better than Monte Carlo, but at a price of larger running times. Unfortunately, the smallest energy values known for LABS ($N \leq 66$) are also far from the typical results from MC and WP, and furthermore, even running both algorithms 1000 times, and picking its best converged result (Optimal MC, Optimal WP) still produce configurations that are far from the ground states for large values of N (see Figure 6).

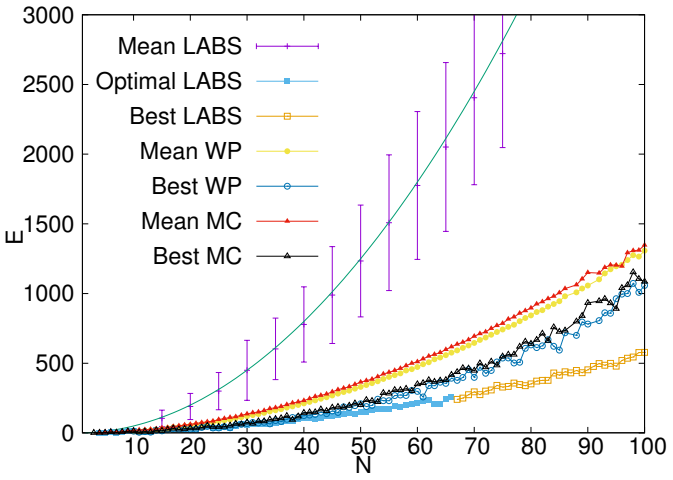

Figure 5. Lowest points are the best known sequences (either known to be the optimal (full squares) or the best guess (open squares)). The highest curve is the mean energy of all the configurations in LABS, and the bars mark the standard deviation from it. Typical solutions from both LABS and MC are well below the typical energies, but still far from the optimal ones. Circles and triangles show the best sequences found by WP and MC in 1000 attempts.

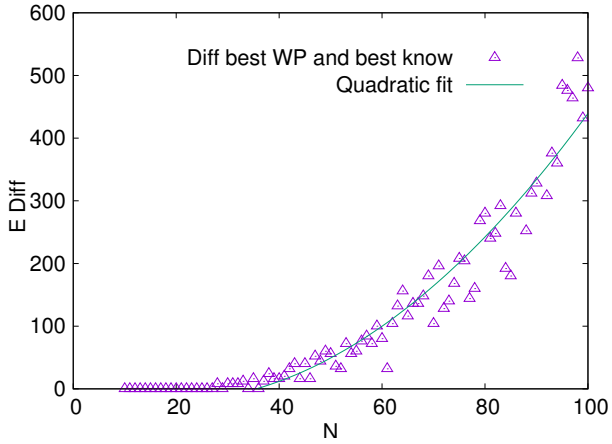

Figure 6. The points represent the energy difference between the lowest energy value in 1000 WP attempts and the best know values reported in the literature. The solid line is a quadratic fit expression $0.08x^2 - 4.7x + 61$.

III. DISORDERED VERSIONS OF LABS

Already in 1994 a series of papers followed a different path [26–28]. They approached the problem borrowing techniques and concepts from the statistical physics of disordered systems, and the model, since then, became a paradigm for the existence of glassy phases in systems without disorder. The idea then was to study a disordered version of the LABS problem and to predict its average properties in the infinite size limit. In short, it is possible to write equation (1) as:

Definition 1. LABS

$$E(S) = \sum_{k=1}^{N-1} \left(\sum_{i,j} J_{i,j}^k S_i S_j\right)^2 \tag{9}$$

where for LABS $J_{i,j}^k$ is defined as:

$$J_{i,j}^k = \begin{cases} 1 & j = i + k \\ 0 & \text{otherwise} \end{cases} . \tag{10}$$

A disordered version of the model [26] may be achieved by relaxing the spatial structure in the autocorrelations $J_{i,j}^k$:

Definition 2. Mean Field LABS

$$J_{i,j}^k = \begin{cases} 1 & \text{with probability } (N-k)/N^2 \\ 0 & \text{otherwise} \end{cases} \tag{11}$$

this is a sort of Mean Field (MF) version of the problem that preserves the connectivity of the variables, but diminishes the correlations between them randomizing $J_{i,j}^k$. Studying such a model it was possible to introduce ideas and methods developed for spin glasses [29] and to find that the system undergoes a first order transition with a glassy phase at low temperatures, much as if quenched disorder was present [26].

Another model, which reminds the original LABS problem, is the anti-ferromagnetic p-Spin model (with $p = 4$) defined by the energy function:

Definition 3. 4-Spin

$$E(S) = \sum_{i,j,k,l} J_{i,j,k,l} S_i S_j S_k S_l \tag{12}$$

where $J_{i,j,k,l}$ is a random diluted matrix with elements 0 and 1 chosen with the same number of interactions than the LABS model.

Although the model is well understood in the diluted and fully connected regimes [30, 31], as far as we know it has never been compared with LABS or its mean field version. The three models share a similar formal structure, defined by a set of binary variables $S_i = \pm 1$ interacting antiferromagnetically in groups of four (mostly). In physics, antiferromagnetic interactions refer to situations where the optimal configuration for the interacting variables is when they avoid having the same value. The arbitrariness of the matrix $J_{i,j,k,l}$ in p-Spin allows for energies $E(S)$ (eq. (12)) with negative values, while in the Mean field and LABS cases (eq. 9), the square guarantees that energies remain positive. The LABS is the most ordered instance of these three models since the groups of interacting variables are not only correlated by the square but also by some spatial structure $j = i + k$ in (10).

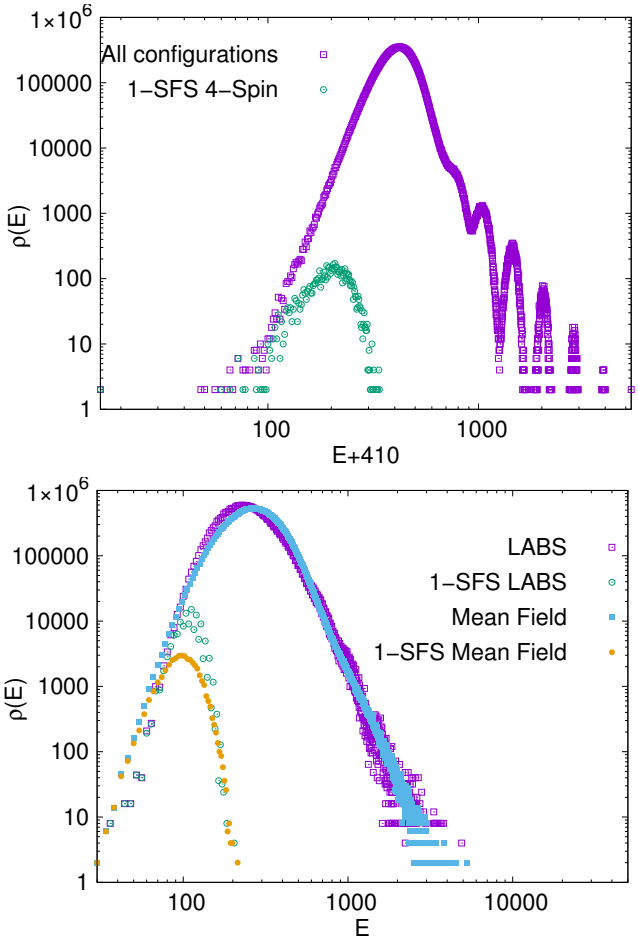

Figure 7. The energy distribution of all the configurations and 1-SFS configurations in the three models p-Spin (top), LABS and MF (bottom). The system size is $N = 25$. There is very similar behaviour between LABS and Mean Field model, the PSpin model exhibit a more rich structure for high energy configurations and allow configurations with negative energy value (note that it has been shifted to fit within a log-log plot).

The greedy Monte Carlo and Warning Propagation algorithm are readily applied to this modified models. An exhaustive enumeration of energies in the configuration space of $N = 25$ models in Fig. 7 exhibit some regularities among the three versions, being LABS and its Mean Field version the most similar. The p-Spin have a richer high energies structure. In all three cases, 1-SFS configurations concentrate in the lower energies range of the spectrum.

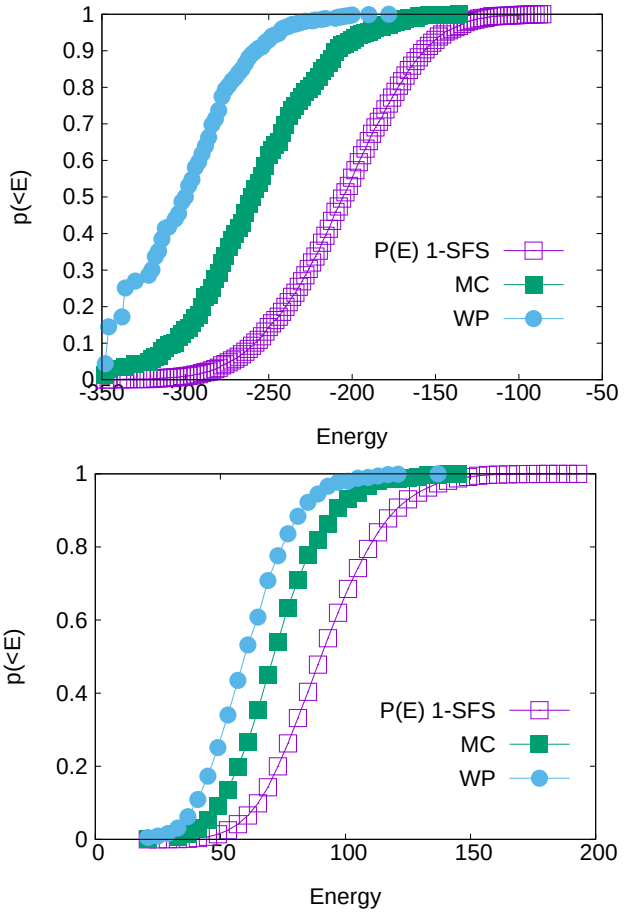

Figure 8. Cumulative distribution of Warning Propagation and Monte Carlo in an $N = 25$ instance of the disordered models p-Spin (top) and Mean Field (bottom). For comparison, the exhaustive enumeration of the 1-SFS configurations is plotted in empty symbols.

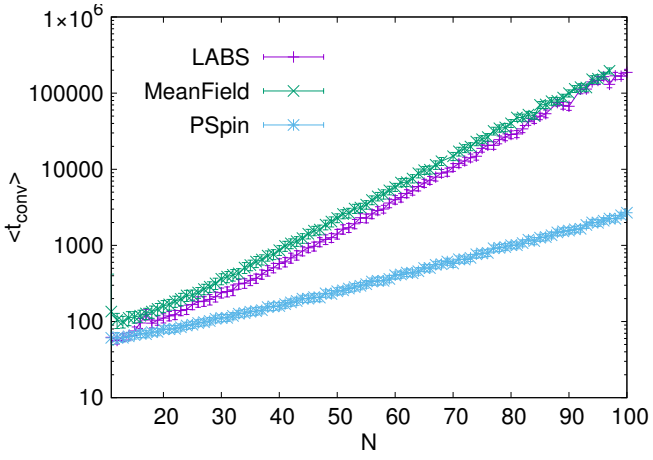

Figure 9. Number of iterations required to reach convergence of WP algorithm on Mean Field, LABS and p-Spin. Each point is an average over 100 runs.

Monte Carlo at T=0 locates 1-SFS states and also (as it did in LABS Fig. 2) samples the lower energies 1-SFS more frequent than the higher ones (see Fig. 8). The behavior of WP and Monte Carlo mark a difference between p-Spin and Mean Field. It seems that the low energy states of p-Spin are more easily accessible by both algorithms than in the Mean Field or LABS cases. This difference suggest that the randomness of p-Spin is somehow simplifying the energy landscape. A supposition that is further supported by the running times of WP in each model, as shown in figure 9, where the number of iterations required to converge in LABS and Mean Field grew exponentially with roughly the same rate, while in p-Spin the growing was with a lower rate, consistent with a simpler energy landscape.

IV. CONCLUSIONS

We have applied two methods ($T = 0$ Monte Carlo and Warning Propagation) to LABS problem. Both methods concentrate in the low energy part of the spectrum of LABS. While Greedy $T = 0$ Monte Carlo converges always (and fast) to 1-SFS solutions, WP generally converges but takes running times that are much larger. On the positive side, WP explore states that are lower in energy than the 1-SFS states of the greedy Monte Carlo.

Unfortunately, both algorithms stuck in a large number of suboptimal fixed points at low energies. Therefore, the lowest autocorrelated sequence remains hard to find for both of them. At the present stage, we only tried to find it by running each algorithm many times from random initial conditions.

We conclude that these two general methods, although simpler, are less powerful than the state of the art optimization techiniques for LABS as those in [1], and fail to give good estimates of the lowest energies for large systems.

To shed some light on this direction we also tried warning propagation on two disordered versions of the LABS problem. While a mean field version of LABS have similar properties to LABS, the p-Spin version seems to be notably easier. This suggest that statistical physics results from p-Spin might not be readily translated to LABS.

Improving over the present work could follow two standard paths in the physics of disordered systems. The first is the use of Survey Propagation algorithm [32] that improves over WP by considering the multiplicity of solutions of WP fixed points. The other would be the inclusion of larger regions in the approximation of the free energy, as is done by Cluster Variational Methods [22, 33, 34], which in this case might be relevant since the basic interactions of the model is between groups of 4 variables. We are currently exploring both.

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