Magnetic problems as a benchmark for genetic algorithm's operators

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Abstract. In the paper it is presented the analysis of results and dynamics of evolutionary optimization applied to the well known magnetic Ising model. The data were obtained using different models and genetic operators and allow to formulate some more general conclusion concerning the possibilities of solving real NP-hard problems propted by physics.

1 Introduction

The physics of magnetism seem to be one of the most extensively studied branches of solid state/material science. This is especially caused by the wealthy of problems concerning the magnetic effects connected to the widely spread applications. Among the topics one can find those with the characteristic size changing by many order of magnitude, from single atom magnetism, through microscopic domains, up to macroscopic samples. Also the number of theoretical and, following them, calculational approaches is vast, matching the scale, complexity and objectives of issue. At the atomic level still the most fruitful attempts are those one pursuing the one proposed by Ising a century ago (as well as its basic level modifications, like Heisenberg or Potts models). Because some main features of it has been shown in earlier works [5] here only the short sketch will be presented.

In the classical Ising-like model we have the set of spins lying in the well defined positions of some structure. One has to point it out that there is no real limitations on the structure considered as well as on the set of possible spin values. The Ising model has been eg. used to calculate properties of such a structure, like, reflecting the small-world properties, Barabasi-Albert network. In the classical attempt the spin set consists two possible states $\{+1, -1\}$ what has been later changed, in order to preserve compatibility with general description to $\{+1/2, -1/2\}$. In such a general view the values of so called z-component of spin vector may vary from minus to plus spin modulus differing by 1 and spin modulus 1 will lead to three state case: $\{+1, 0, -1\}$. The interaction between spins is described by the simple formula giving the total energy of the system:

$$H = -J \sum_{ij} S_i S_j - h \sum_i S_i. \tag{1}$$

Certainly this model is not adequate for real materials and for the case of them a lot of different additional terms depending on particular atom character may be added. This is however sufficient for performing some tests enabling the comparison of different

evolutionary operator's influence on the efficiency of calculation understood as a time needed t obtain the best result. We should also remark that an attempt to perform some more systematic calculations for basic model were strongly influenced by difficulties with solving much harder problem like ternary alloys [5, 7].

2 Some existing approaches

Magnetic models based on the Ising attempt are used not only in pure magnetism but they work also as a benchmark for different types of study like sociophysics, phase transition study and percolation or some basic models of cellular automata evolution. They are also the test areas for various calculational procedures especially those one which are based on discrete configurational space. Therefore one can look at them from two points of view. One of them is strictly physical: we are just looking for the best solution of physical problem described by the interaction similar to those presented in equation 1. The second one is the attempt to use well defined system to test some computational procedures and their features. The connection between Ising-like system and the Evolutionary Algorithm is apparent as one considers the system analysis to be the optimization problem.

Concerning the physical interest one can divide the areas of use into few groups.

Ground state calculations In this group we will name the calculations devoted to study the problem as it is defined by the equation 1. Actually we can list here only the basic work of Anderson [1] where the twodimensional Ising model was solved for the first time for the ferromagnetic coupling and the attempts presented earlier at the KAEiOG conferences [5, 7]. These topics, concerning the of complex structures optimization, are indeed the most promising direction of ground state study.

Thermodynamical calculations We can also regard the calculation of system properties in the given temperature as the optimization problem. The minimization concerns here not the total energy but the Gibbs free energy, see formula 2. The main problem is here the way to calculate the entropy of system S. In further part of this paper we will spend a little more time on this problem. When talking about such problems one has to list few papers devoted to study 2D Ising model [10, 6].

Spin glasses Although the calculation for spin glasses generally belong **Spin glasses** Although the calculation for spin glasses generally belong to the first group because they deal with the problem of ground state searching, due to the character of sample we decided to extract it and present as a separate group. In the spin glasses the exchange constants J are sampled from the initially assumed distribution. The primary attempt was presented by Sutton et al. [14] but the most important step was Hartmann's cluster-exact approximation [8, 9]. Quite recently this method was in detail studied by Blum and coworkers [3].

3 Model

In this paper we deal with the classical two-dimensional Ising model, ie. two-state ($\{+1, -1\}$) system on the square lattice of size L. The goal is to minimize Gibbs free energy of the system and to obtain the temperature characteristics related to the magnetic phase transition. We are interested in the shape of magnetization curve, ferro-

paramagnetic transition temperature (T_C), the values of critical exponents describing the process of reaching T_C point. The choice of basic Ising model was substantiated by two major objectives. During former KAEiOG conferences we reported the problems with minimizing the complex system of ternary alloy [5, 7]. These problems led us to such an effort to perform more systematic investigations on the simplified model. Although the calculations for Ising model with the help of EA has been presented [6] we decided to come back to it and make some tests which could answer the questions about the dependence of efficiency on size, entropy model, optimization point (understood as a point on the phase diagram) or, especially, evolutionary operators used. The selection of Ising model was caused by the fact that it is well known, indeed this is the only low-level magnetic problem solved analytically, so the results can be easily compared with the exact solution.

Let us now summarize main features which distinguish different results across this paper. The first one is the model of entropy. Using formula

$$G = U - TS \tag{2}$$

(U is the internal energy calculated using hamiltonian H) we have to identify the usual, thermodynamical meaning of entropy with the configurational one. Such an approach is widely accepted in physics [11, 12, 13, 4, 16, 2]. In this paper two possible methods were used. The Bukman's pair approximation [4] follows the reduction of cumulant series to the first two terms and uses the single-site and pair densities (ρ_1, ρ_2) to calculate entropy per one site as:

$$\sigma = \frac{z}{2}\sigma_2 - (z-1)\sigma_1, \tag{3}$$

σ_1 and σ_1 are calculated from densities according to the usual Boltzmann-Gibbs formula:

$$\sigma_1 = -k_B \sum_i \rho_{1,i} * ln(\rho_{1,i}), \quad \sigma_2 = -k_B \sum_i \rho_{2,i} * ln(\rho_{2,i}) \tag{4}$$

The calculations made using this model will be denoted **E1**.

The results of pair approximation are compared to those obtained using so called Tsallis entropy [15], denoted **E2**.

$$\sigma = k_B \frac{1 - \sum_i \rho_i^q}{1 - q} \tag{5}$$

The idea of entropy redefining is the effect of analysis of its nonextensivity resulting eg. in the size effect. For simplicity we took into account only the most simple single-site formula what makes it possible to connect it directly with magnetization. One has to notice that Tsallis model has the parameter q which choice can significantly change the properties of studied system. On the fig.1 there is presented the comparison of analytical magnetization curve of pure Ising model with those obtained by minimization using mentioned entropies with different parameters.

Please, notice that we will not discuss here the physical correctness of proposed approaches. Although the pair approximation with Boltzmann-Gibbs entropy is well justified, the use of single-site Tsallis model is hardly accepted as a true physical solution. As the best illustration we can call so called ANNNI (Axial Next Nearest Neighbour Ising)

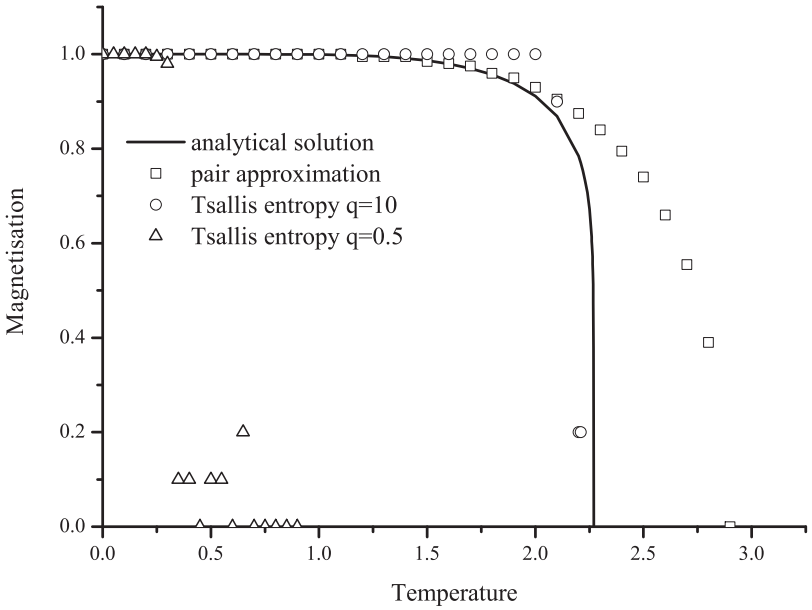

Figure 1. The magnetization in the Ising model.

model where the nn interaction is of ferromagnetic and the nnn - antiferromagnetic character. The samples of this type exhibit interesting behaviour with a lot of different possible states on the phase diagram leading to zero magnetization. It doesn't exist eg. the most simple ferromagnetic ordering but spins are organized in chains with the same orientation, like $< 2, 2 >, < 3, 3 >, < 3, 2, 2 >$ or generally $< 3^n, 2, 2 >$. The quantities in braces means the numbers of successive spins with the same direction. Apart from the model of entropy used it is obviously impossible to distinguish these states with single-state calculation.

	S1M1	S1M2	S1M3	S2M1	S2M2	S2M3	S3M1	S3M2	S3M3
FE1: $\bar{n}$	310.5	304.6	310.5	304.9	310.5	297.3	304.9	316.3	308.5
s_n	282.5	276.8	282.5	267.5	282.5	275.8	267.5	319.3	270.7
FE2: $\bar{n}$	296.9	278.2	311.0	279.5	278.2	313.0	281.5	308.7	311.3
s_n	298.5	272.1	299.9	272.6	272.1	299.8	296.8	299.9	299.4
PE1: $\bar{n}$	56.7	60.4	82.2	60.4	60.7	84.1	83.9	82.2	82.2
s_n	61.1	55.4	86.3	55.4	56.2	86.9	88.5	86.3	86.3
PE2:	8.3	8.5	8.6	8.3	6.9	5.0	6.9	6.8	5.1

Table 1. Results of optimization. The first row of every cell presents the average number of generation when the minimum was reached. The lower row contains the value of standard deviation. The exception is for the PE2 type of calculation where, due to computational hardess, there is presented the percentage of runs which led to global optimum in 10^4 generations.

The second important point is the selection of temperature which corresponds to the choice of the point on the phase diagram. We chose two temperatures in order to cover the regions characterized by ferro- as well as paramagnetic ordering. We avoided the selection of the most imposing $T = 0$ point because we wanted to have a nonzero influence of entropy. Therefore the temperature $T = 1$ was chosen and these calculations are described by **F**. As a paramagnetic point (**P**) was indeed selected the point just before the phase transition $T = 2.1$ where the magnetization has already fallen from the $m = 1$ value but wasn't also really paramagnetic.

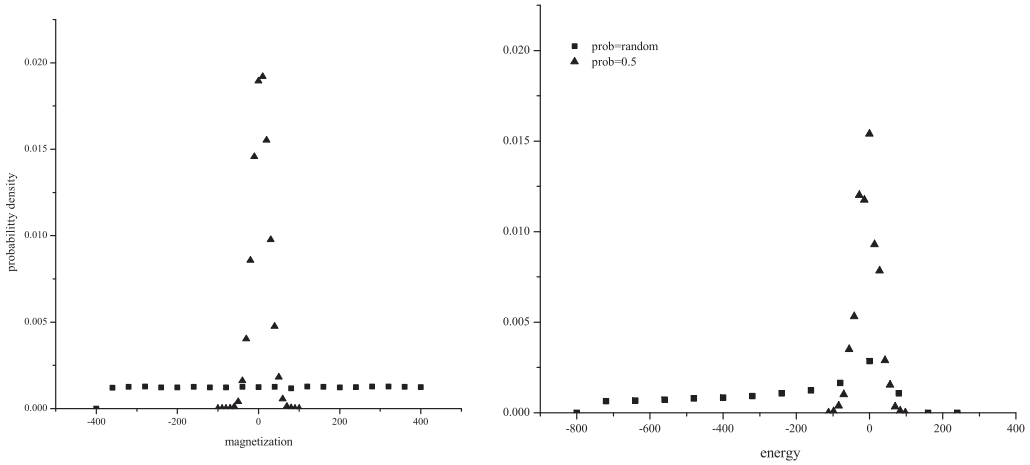

Figure 2. Initial distributions of magnetization and energy for two ways of initial values setting.

Concerning the true evolutionary operators we decided to compare three most popular selection algorithms: roulette wheel(**S1**), tournament with three competitors (**S2**) and the rank selection(**S3**). Mutation was performed as spin flip performed on a random spin from the chosen individual from the population. The mutation rate is then understood as a percentage of individuals for which only one flip is performed. As for selection also here three possible values were selected: 0.1((**M1**), 0.2((**M2**), 0.3((**M3**). Considering that the size of population was taken to be 100 for **E1** and 50 **E2** at every stage of new generation creation 10,20 or 30 (5,10,15) offsprings respectively undergoes random mutation. Only the best individual, according to the preferred elististic model, is just copied between the old and the new one generation and isn't modified by genetic algorithms.

The objective function is selected typically for the energetic problems:

$$f(U) = \exp\left(-\alpha \frac{U - U_{min}}{U_{max} - U_{min}}\right), \tag{6}$$

where U_{min} and U_{max} are the lowest and the highest free energy value in population, the selectivity parameter α was set to 1. One should also point out that no process of local optimization was performed.

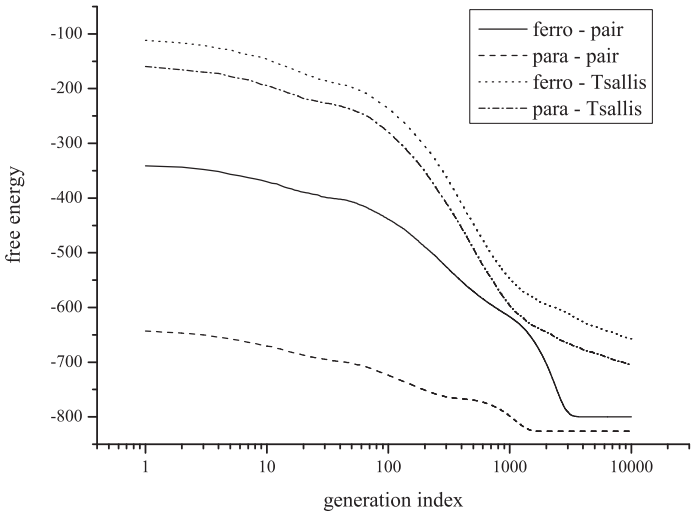

Figure 3. The plot of average free energy dependence on the generation index, averaged over a number of runs.

4 Results and Conclusions

The results of optimization are presented in table 1.

The efficiency of ferromagnetic ordering seems to be almost totally independent on the optimization parameters. For pair as well as Tsallis entropy, for different types of population update the results are versy similar, one can say the same. The average time of reaching minimum $\bar{n}$ is always about 300 generations. What is interesting that the standard deviation value is of the same order this number what suggests the existence of long tails in the $\bar{n}$ distribution. The comparison which is not shown here for the lack of place makes it possible to remark that evolutionary operators are negligible when looking for the crucial time consuming factor. Independently of their combination the time spent on calculations is similar and the most important factor remains the physical part of calculations. Interesting differences appears during comparison of data for paramagnetic region. Although for **E1** if becomes more efficient, for **E2** the procedure starts to diverge. It is especially strange due to the fact that for single-site Tsallis model the entropy is better defined and connected simply to magnetization.

One should mention also the initial selection of population as an significant factor influencing the optimization run. In the calculations presented above the determination of initial direction of every spin needed two samplings. For every spin the individual probability of being directed up or down is sampled from the uniform distribution $[0, 1]$. Then the direction of spin is finally determined on the basis of comparison of newly sampled random with this probability. We tried also to use the second mechanism where every spin has just the same probability (in our calculations 1/2) to be set in one of two possible directions. The differences in the shape of initial energy (not the Gibbs free energy) and magnetization distributions are shown on fig.2. The plots obtained using second method are visibly narrower thus should lead to the better results for the

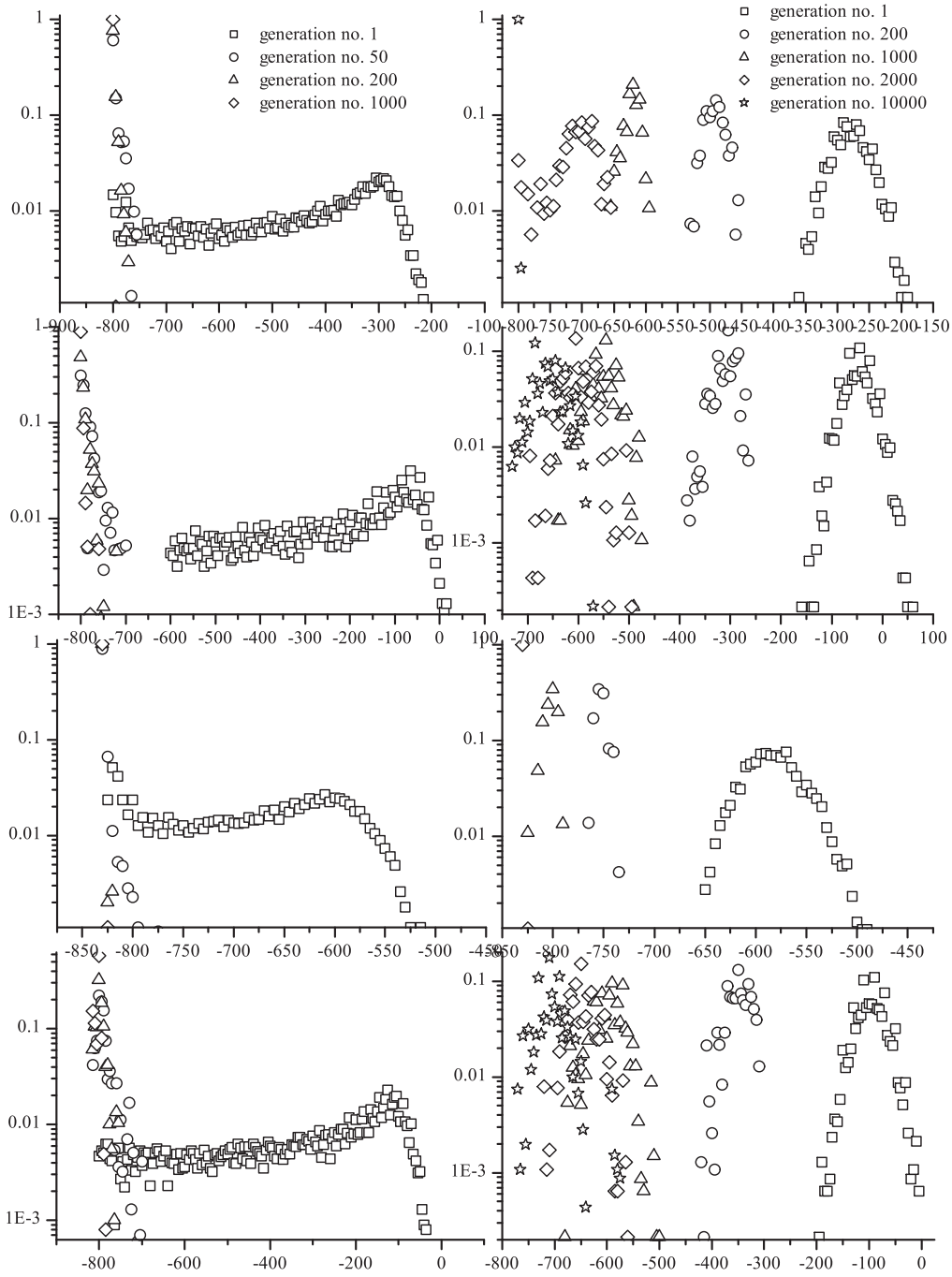

Figure 4. Free energy distribution in different generations. Columns correspond to the method of initial population selection: left - totally random, right - $p = 1/2$. In successive rows there are different types of simulation: 1 - **FE1**, 2 - **FE2**, 3 - **PE1**, 4 - **PE2**.

paramagnetic case. This observation is hovewer not confirmed in calculations.

We tried also to study in two ways the dynamics of optimization. Figure 3 presents the average free energy in the population when started from the initially equilibrium distribution of up and down spins. Certainly this plot cannot be directly compared to the results from table 1 where the first existence of minimum is grabbed. It gives the information about the diversity of population. It is interesting that for the pair approximation quite fast the populations become uniform. There is no additional, except of mutation, mechanism leading to artificial differentiating. For the same population index, populations obtained using Tsallis entropy are, in spite of smaller set of acceptable values still diversified.

Figure 4 shows the free energy distribution for selected generations in the logarithmic scale. The difference which is seen already in the initial generation, promotes to the next ones, even thousands later. The distributions for totally random sampling are asymmetric with maximum for higher energies and almost already after genetic procedure starts the maximum of distribution shifts to the value of global minimum. For $p = 1/2$ the plots are symmetric and this symmetry is observed for all generations even when the global minimum is reached.

Summarizing, we want to underline that for the case of NP hard problem of magnetic system minimization the crucial problem is rather the physical description and the sensible choice of initial conditions not a form of evolutionary operators. This, sharply simplified, conclusion is true for the basic magnetic model and its extension to the models where also the form will be of great importance, can make the solution hard challenge.

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