Application of heuristic optimization techniques
in physics of magnetism

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Abstract

The progress of technical abilities of computers creates enables the use of still more elaborated computational techniques. The classical examples are here the Monte-Carlo or the Molecular Dynamics simulations which are the sensible alternative to study even quite complicated structures. In this work we want, however, to deal with the problems which may be described as the optimization questions and from the algorithmical point of view are NP-hard problems. The typical problem studied is here the searching for the ground states of different magnetic systems. In the presented paper we pay the attention to the samples described by the Ising hamiltonian and want to show the use of evolutionary algorithm not only in finding the ground state but also as a tool to look for the minimum energy state at different temperatures.

1. Introduction

Physics offers to people dealing with algorithmical problems a great number of possibilities. From one point of view it offers a lot of problems which are computationally hard and may act as a good testing area for new numerical techniques and on the other hand it may influence the emergence of new ways of problems solving. The crucial example of widely spread idea of physical origin is the simulated annealing which comes from the Metropolis' work on equation of state calculations.

In this paper only a small area of the above mentioned applications will be presented. We want to focus first of all on the problems of optimization understood as a finding minimum or maximum value of some parameter characterizing the physical system or the result of measurement performed on it. Certainly there can be numerous ways of approaching these problems but the usual discrimination is into the two classes of problems, those which can be solved using local optimization techniques and those which need an alternative method. Whereas the local optimizations are usually based on classical deterministic methods like Newton-Raphson, conjugate gradients or even simple

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gradient, the second set of problems is inaccessible for this well-defined type of computation. The main reason for it is the multidimensionality of search space and the existence of a lot of locally acceptable solutions described in the language of basins of attraction. This causes the necessity of using the randomized heuristic methods.

Currently a lot of methods of global optimization are used. They are, however, based on a few basic methods and detailed solution is usually slightly specialized to follow the requirements of the problem studied or hybridized to fully exploit the advantages of a few methods. Among the most frequently used global optimization techniques one should mention: Simulated Annealing, Genetic (Evolutionary) Algorithm, Taboo Search or Ant Colony Optimization. Because the last two methods are suitable rather for discrete problems in the most physical applications it can be found either SA or GA or the mixture of both them.

The GA technique which is the point of interest of this work has been, very widely used to study different issues for about ten years. It should be pointed out that the method itself is much older. It was proposed independently by two authors [2,3] but its rapid progress is connected mainly with the growth of power of computers required by the relatively big amount of memory and a large number of calculations performed during the optimization process. The short sketch over its application in the area of physics has to enclose such different fields like superconductivity [4], geophysics [5], surface reconstruction study [6], quantum mechanical calculations of semiconductor microstructure [7] or analysis of experimental data from X-ray spectrometry [8,9] and LEED [10].

A very specific area of global optimization in solid state physics is the determination of cluster structures due to its clear understanding as a energy minimization process. The crucial role is played here by the interaction potential which allows to try to find the minimum energy for such different structures as water clusters [11], metals [12,13], fullerenes [14].

In this paper we focus on the application of global optimization methods to magnetic systems. Its construction as a set of well defined values (or values from well defined interval) distributed on the n-dimensional cubic cellular net has an effect on almost ideal transformation to the data representation needed by the genetic algorithms. Considering the well known Ising model in which we have only two types of spin we may notice that simple mapping onto {0,1} the set of values allows to use the classical GA with the binary representation. Certainly for the most complicated systems this historical approach is not sufficient but the discretization of configuration space as well as possible single cell states enables simple application of this method.

The genetic approach to magnetic problems started with the work of Anderson and et. al. devoted to the optimization of ground state of ferromagnetic system[15]. Since then the studies have followed a few directions. One of them

is the analysis of ground states of samples especially those described by more complicated spin interaction like spin glasses characterized by randomized exchange constants and thus leading to antiferromagnetic coupling. The seminal works come in this topic from Hutton et al. [16] and Hartmann[17]. From the paper of Maksymowicz et al. [18] a less developed branch concerning the thermodynamical study of magnetic models started. This work also belongs to this group.

2. Basics of optimization procedure

Consider the d-dimensional simple cubic Ising sample i.e. the system described by the following assumptions. In each of the L^d positions (where L is the linear size of the sample) there can be stored one spin with the discrete set of values
{-1,+1}. Certainly these values reflect the only two possible states of spin: up and down. The internal energy of this system is described by the simplest Ising interaction hamiltonian:

$$H = -J\sum_{ij} S_i S_j .$$ (1)

As it can be seen in our calculations only the interaction with the nearest neighbours, as was proposed in the original paper by Ising. A few elements which are usually present in the contemporary models are omitted here like the next-nearest neighbour interactions, biquadratic or anisotropic terms or the influence of external field. However, this simplified approach makes it possible to compare the results with those obtained in the other type of calculations including the analytical ones obtained by Onsager. The exchange integral J was chosen positive in order to have ferromagnetic material (J = 1).

The crucial point in the thermodynamical calculations is that we do not need to minimize the internal energy but the Gibbs free energy, which is related to the temperature through entropy:

$$U = H - TS .$$ (2)

The entropy calculation will be performed according to the approximation proposed by Bukman [19] and applied by Balcerzak [20] based on its expansion into a series of cumulants:

$$S = \sum_i \tilde{\sigma}_i + \sum_{ij} \tilde{\sigma}_{ij} + \sum_{ijk} \tilde{\sigma}_{ijk} + ...$$ (3)

which has to be obtained from the Shannon entropies calculated for the respective n-spin term. Whereas the detailed description of the algebra used may be found in the seminal works here only the most important features of this approach will be briefly presented. The relation between the n-spin entropy and the n-spin cumulant is as follows:

$$\sigma_i = \tilde{\sigma}_i,$$
$$\sigma_{ij} = \tilde{\sigma}_i + \tilde{\sigma}_j + \tilde{\sigma}_{ij}, \qquad (4)$$
$$\sigma_{ijk} = \tilde{\sigma}_i + \tilde{\sigma}_j + \tilde{\sigma}_k + \tilde{\sigma}_{ij} + \tilde{\sigma}_{ik} + \tilde{\sigma}_{jk} + \tilde{\sigma}_{ijk},$$

where

$$\sigma_i = -k_B \left\langle \ln \rho_i \right\rangle,$$
$$\sigma_{ij} = -k_B \left\langle \ln \rho_{ij} \right\rangle, \qquad (4)$$
$$\sigma_{ijk} = -k_B \left\langle \ln \rho_{ijk} \right\rangle.$$

After rejecting the higher order terms and restricting the calculations to the second term corresponding to the pair approximation there can be performed the summation over all single spins and pairs of spins leading to the formula:

$$S = N \left(\frac{z}{2} \sigma_2 - (z-1) \sigma_1 \right). \qquad (5)$$

When compared to the earlier formulas some simplifying replacements have been made here: $N = L^d$ is the number of spins, $\sigma_i \rightarrow \sigma_1$, $\sigma_{ij} \rightarrow \sigma_2$ and z is the number of nearest neighbour which for the sc sample is equal to $z = 2n$. The approach presented above allows to determine the minimum free energy configuration for the given temperature expressed in k_B units and as a result other characteristic features like phase transition point. The details of the procedure leading to the phase transition temperature determination are not presented here, the reader can find them in [21].

In the calculations we used the population formed by 50 individuals in the real number representation. This is certainly a different approach as compared with the bit representation described earlier, but it is more general thus allowing to study more complicated spin systems with the same code. It does not also exceed even for quite great samples the technical properties of computer and can save some time usually devoted to the process of decoding of bit string. In the selection phase the elitistic, exponential function of the form known from the cluster calculations is used:

$$fit(\Omega) = \exp\left(-\alpha \frac{G(\Omega) - G_{min}}{G_{max} - G_{min}} \right). \qquad (6)$$

3. Results and conclusions

Let us initially concentrate on the two-dimensional sample and compare the results obtained using the evolutionary optimization with well known theoretical solution. It is presented in Fig. 1, where the dependence of order parameter m identical with magnetization at the temperature is presented. The solution obtained about 60 years ago by Onsager is presented as a solid line. The plots shown in this figure lead to some general conclusions. First of all, the utility of

this method when applied to simple magnetic systems is confirmed. The phase transition point is easy to determine, however, it lies distinctly higher than the theoretical one. It should be stressed that this behaviour may be easily explained as the effect of pair approximation used to calculate the entropy. Because this simplest model may be also studied analytically, and such calculations have been recently performed [20], it is possible to compare our results with them ones. This comparison is not presented here but the main result interesting from the point of view of our calculations is that pair approximation adapted to the 1/2 spin systems produces an overestimated result for the critical temperature. So the result itself is physically not interesting but the model is an interesting testing tool for evolutionary algorithm implementation.
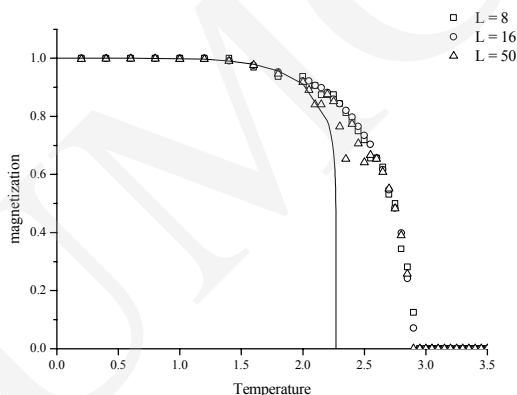

Fig. 1. The temperature dependence of magnetization for the two-dimensional Ising model
in the pair approximation. The absence of size effect is visible. Solid line corresponds
to the correct solution and Tc = 2.269

The more interesting feature comes from the comparison of sets of points obtained for different sample sizes. The usual effect in the simulations of thermodynamical processes is the existence of size effect, which leads to scaling of as well phase transition temperature as critical coefficients. This feature is not observed on our plot although the sizes of samples (L^d) are modified in a range of one order (256-2500).

The next plot presents the magnetization dependence on temperature for the samples with different dimensionality. Because of the above mentioned lack of relation between the size of sample and the magnetization shape curvature relatively small systems were chosen (d = 2, L = 16, N = 256; d = 3, L = 12, N = 1728; d = 4, L = 6, N = 1296).

Although everyone at least a little familiar with the problems of magnetism can enumerate some samples which can be described as a one-dimensional spin

chain or a flat 2D system and three dimensions if the usual dimensionality is to
study the real problems , the calculation for d = 4 seems to be useless. Such an
opinion is, however, not valid for a few reasons. The Ising model and its
modifications are a very popular area to test a lot of attempts designed for the
phase transition study. The dimension d = 4 is a special value for these
investigations because this is so called upper critical dimension. For the samples
with all dimensionalities higher than UCD the critical coefficients should have
the same value.

Studying the critical properties of d-dimensional Ising sample we will focus
on the critical exponent β which is defined according to the well known formula:

$$m = (T_C - T)^{\beta} \tag{7}$$

and describes the behaviour of order parameter in the vicinity of phase transition
temperature.

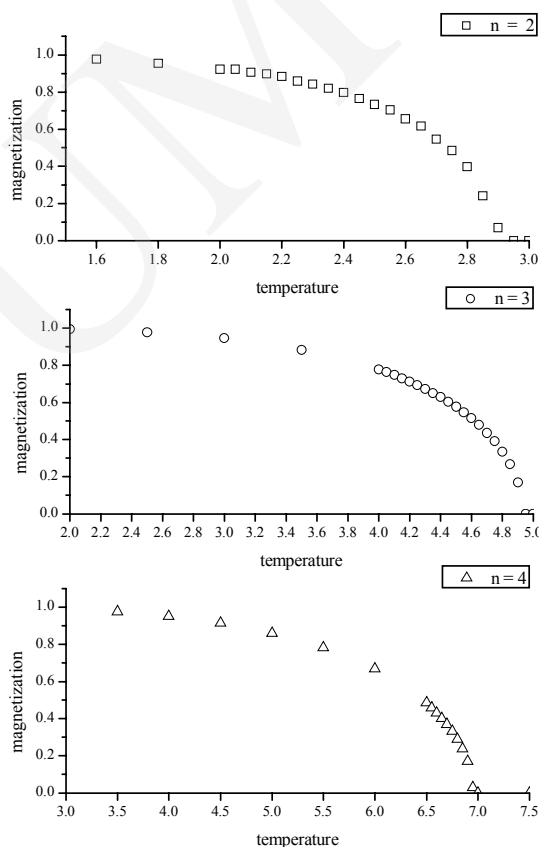

Fig. 2. Magnetization dependence on temperature for the samples with different
dimensionalities (d = 2,3,4)

All plots shown in the above figure present the similar behaviour: the overestimation of critical temperature and the change order parameter dependence character leading to incorrect value of β. The values from the analytical or simulational solutions are compared with those obtained in our optimization.

Table 1. The critical properties for two-,three- and four-dimensional Ising model obtained using the evolutionary optimization for pair approximation

	critical temperature				critical exponent β	
	other sources	EA	difference	relative difference	other sources	EA
n = 2	2.27	2.85	0.58	25.50%	0.125	0.63
n = 3	4.53	4.92	0.39	8.60%	0.30	0.55
n = 4	6.68	6.95	0.27	4.04%	0.50	0.85

A few observations concerning the critical values can be made. The phase transition temperature is for all calculations overestimated but it should be pointed out that this difference decreases with dimensionality as well in absolute as in relative scale reaching for $d = 4$ value only about 4%. It would be an interesting question how this difference will behave for the samples with the dimensionalities exceeding the upper critical dimension.

One should look at our results from a few different points of view. The first is the physical one where the entropy calculations are very interesting. Evolutionary computations are a tool which can overcome some difficulties with applying higher order corrections to entropy expansion. This is certainly due to its character as a "brute force" method. The code dealing with the three-spin interaction cumulant in the Bukman's expression is now in the phase of tests. From the point of view of algorithmics and algorithm testing the use of discrete magnetic systems with more complicated structure (like triangular systems) interaction function or (like spin glasses or samples with other types of interaction included) may be very interesting and helpful.

It can be also stressed that the model presented is very hard when treated as a subject of local minimization due to complex character of entropy calculations. This difficulty will increase with the increasing order of Bukman's expansion. So the method has to generate the optimum without any help coming from possible hybridization of the method.

I think one can say that the approach presented here is an efficient one. The size of search space for the studied samples with about 1000 spins may be established approximately as 10^{300} configurations. The optimum is usually found during the first thousand of generations only for greater systems sometimes it needs more time. However, during a lot of independent runs there has never been a situation when the minimum would not be found through 2000 generations. This result depends rather on the initial population sampling then on

the complexity of problem. The calculation time for the greatest configuration ($d = 2$, $L = 50$, $N = 2500$) was only slightly greater than 10 minutes when performed on the single Pentium 2.6G processor.

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