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# EXACT GROUND STATES OF ISING SPIN GLASSES: NEW EXPERIMENTAL RESULTS WITH A BRANCH AND CUT ALGORITHM

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This work was partially supported by EEC Contract SC1$*$-CT91-0620 (DTEE).

**Abstract**

In this paper we study 2-dimensional Ising spin glasses on a grid with nearest neighbor and periodic boundary interactions, based on a Gaussian bond distribution, and an exterior magnetic field. We show how using a technique called branch and cut, the exact ground states of grids of sizes up to $100 \times 100$ can be determined in a moderate amount of computation time, and we report on extensive computational tests. With our method we produce results based on more than 20 000 experiments on the properties of spin glasses whose errors depend only on the assumptions on the model and not on the computational process. This feature is a clear advantage of the method over other more popular ways to compute the ground state, like Monte Carlo simulation including simulated annealing, evolutionary, and genetic algorithms, that provide only approximate ground states with a degree of accuracy that cannot be determined a priori. Our ground state energy estimation at zero field is $-1.317$.

*Keywords:* branch and cut, Ising spin glasses, exact ground states

## 1. Introduction

Finding the ground state properties of Ising spin glasses is an important problem in physics. The Ising model is one of the most commonly used, both for its simplicity and its accuracy in representing real problems.

The configurations that are mostly considered in the literature are the two-dimensional Ising spin glasses on a grid with nearest neighborhood and periodic boundary interactions, and an exterior magnetic field. The periodic boundary conditions are a standard way of approximating an infinite planar spin glass with a structure that contains only a finite number of spins.

Unfortunately, there are no partition functions in closed form that, given all interactions between the spins and the exterior field, yield a ground state. Therefore, the only way to compute a ground state is using a numerical algorithm. Since the total number of states for a structure with $n$ spins is $2^n$, as soon as $n$ exceeds 30–35, it is impossible, from a computational point of view, to find a ground state by *brute force*, i.e., by enumerating all possible states and computing the energy for each of them.

A fundamental question from both a practical and a theoretical point of view in computational mathematics is to determine whether it is possible to design an algorithm that, for any possible choice of the spin interactions and of the magnetic field, finds a ground state in a number of elementary operations bounded by a polynomial function of $n$, or, more precisely, of the number of bits needed to store the problem data. A problem for which this is possible is called *polynomially solvable* and the procedure used is called a *polynomial algorithm.*

The theory of computational complexity has given quite negative results for the possibility of solving the Ising spin glass with periodic boundary conditions with a polynomial algorithm. The only case for which a polynomial algorithm has been found is for the $\pm J$ model with no magnetic field [3]. For the Gaussian case the question is still open, while as soon as we have an exterior field, the problem becomes $\mathcal{NP}$-hard for all kinds of spin interactions. When a problem is proved $\mathcal{NP}$-hard, it is generally considered as notoriously hard, and it is believed that there can be no polynomial algorithm for its solution.

Due to the difficulty of the problem, the most popular methods described in the literature compute an approximation of the value of the minimum energy of the spin glass. Such methods usually use Monte Carlo simulation including simulated annealing [14], [20], evolutionary [22] and genetic algorithms [12], [23]. Two of the main drawbacks of these heuristic methods are:

(1) It is not possible to estimate how far the produced solution, when the algorithm stops, is away from a real ground state. Therefore it is not possible to determine reliably the degree of accuracy of the experimental results produced with these methods. For example, if we want to compute the expected ground state energy as a function of the grid size, using heuristic methods, the values will always have a positive bias, no matter how large the grid size is, how many experiments are made, and how much computation time is invested.

(2) Two different states with almost the same energy may be completely different. Therefore, the state produced by one of these algorithms cannot yield any useful information on the structure of the ground state; consequently these methods are completely inadequate when *real* ground states have to been analyzed as, e.g., in protein folding, as was observed in [17].

Only few authors have reported on computational results for methods that compute exact ground states. The polynomially solvable case of planar grids with no periodic boundary conditions and no magnetic field is treated in, e.g., [1], [7], and [8], instances for which no polynomial algorithm is known are treated in, e.g., [5], [11], and [18]. The most recent results for planar grids with periodic boundary conditions and exterior magnetic field, in which the interactions are taken from a Gaussian distribution — the case we want to concentrate on in this study — are given by Barahona [4], in which he uses a "primal" cutting plane algorithm in order to study the ground state magnetization as a function of the magnetic field, a task that requires an exact algorithm due to (2) above. The described implementation can handle grids with sizes up to $35 \times 35$, for which the computation took about 14 hours on an IBM RISC6000 workstation. Barahona [4] states: "... we do not have a good bound for the amount of time that it would take for the worst possible instance. Also, we do not expect to be able to handle considerably larger grids, on this type of workstation.". Nevertheless, polyhedral approaches, a "primal" one, as used in this reference, and a "dual" one, as described previously in [5], [11], have given the most promising results.

A more sophisticated implementation of the "dual" method described in [5], [11] (which we would prefer to call "primal/dual" for reasons which go beyond this exposition), with an additional enumerative frame, on a comparable workstation, enabled us to handle $100 \times 100$ grids in moderate computation times. Therefore, we can give computational results based on more than 20 000 samples. However, we agree that it is hard to predict the running time, as our computational study will indicate below. Indeed we can solve single instances of much bigger size, say $150 \times 150$, but the variance in running time for different instances is so high, that we cannot run such sizes routinely.

## 2. Ground states and maximum cuts

Finding the ground state of a spin glass is a problem very much related to a well known problem in combinatorial optimization: the maximum cut problem in a weighted graph (max-cut problem for short).

The max-cut problem is the following. We are given a graph $G = (V, E)$ with weights $c_{ij} \in \mathbb{R}$ for all edges $ij \in E$. For each (possibly empty) subset $W$ of the node set $V$, the cut $\delta(W)$ of $G$ is the set of all its edges with one endpoint in $W$ and the other in $V \backslash W := \{i \in V \mid i \notin W\}$. The weight of a cut is given by the sum of the weights of all its edges. The max-cut problem is to find a cut of $G$ with maximum weight.

Assume that we have a spin glass with $n$ spins $S_1, S_2, \ldots, S_n$ and a uniform exterior magnetic field $S_0$ with strength $h$. We set $V = \{0, 1, \ldots, n\}$ and consider $V$ as the node set of a graph $G = (V, E)$, the interaction graph associated with the system. For a pair $i, j$ of nodes, $G$ contains an edge $ij$ if the interaction $J_{ij}$ between two magnetic impurities (or between the field and one impurity) is nonzero. For symmetry reasons the "ghost spin" variable $S_0$ corresponding to the field may be fixed, say to $S_0 = +1$. Given a spin configuration $\omega$, the value of the energy is

$$H(\omega) = -\sum_{ij \in E} J_{ij} S_i S_j - h \sum_{i=1}^{n} S_0 S_i.$$

Observe that each spin configuration $\omega$ induces a partition of the node set $V$ of the interaction graph $G$ into node sets $V^+$ and $V^-$, where $V^+ := \{i \in V \mid S_i = +1\}$ and $V^- = \{i \in V \mid S_i = -1\}$. So the energy of the spin configuration $\omega$ can be translated to the form

$$H(\omega) = -2 \sum_{ij \in \delta(V^+)} c_{ij} - C,$$

where $c_{ij} := -J_{ij}$ for all $ij \in E$ and $C := \sum_{ij \in E} J_{ij}$. Hence, the problem of minimizing $H$ is equivalent to maximizing

$$c(\delta(V^+)) := \sum_{ij \in \delta(V^+)} c_{ij}$$

over all $V^+ \subseteq V$.

This problem is a weighted max-cut problem in the interaction graph $G$ associated with the spin glass system. Thus, finding a ground state in the Ising model of a spin glass is equivalent to finding an optimum solution of the corresponding max-cut problem. The standard 2-dimensional grid model with nearest neighbor interactions, no periodic boundary conditions and no magnetic field leads to the problem of solving a max-cut problem in a planar graph.

For planar graphs, Orlova and Dorfman [19] and Hadlock [13] have found a polynomial time algorithm. The 2-dimensional grid model with periodic boundary conditions leads to the max-cut problem for the interaction graph $G$, which is embeddable on the toroidal sphere. For all toroidal interaction graphs, provided interactions have value $\pm J$ and there is no field, Barahona found a polynomial time algorithm [2]. But for practical purposes this algorithm is not useful since the running time is proportional to $|V|^7$. In the Gaussian model with zero field, no polynomial time algorithm is known, and it is not clear if there exists one. However, Barahona showed that for the 2-dimensional grid model with nearest neighbor interactions and a magnetic field the problem is $\mathcal{NP}$-hard, even if there are no periodic boundary conditions [3]. Computational studies for this case have been carried out in [21].

## 3. Branch and Cut

We will first describe the theoretical background of our method. It is based on ideas of polyhedral combinatorics. Suppose a graph $G = (V, E)$ with edge weights $c_{ij}$ for $ij \in E$ is given. We associate with $G$ the real vector space $\mathbb{R}^E$, where the components of the vectors are indexed by the elements of $E$. For each cut $\delta(W)$, $W \subseteq V$, we define its incidence vector $\chi^{\delta(W)} \in \mathbb{R}^E$ by setting $\chi_e^{\delta(W)} = 1$ if $e \in \delta(W)$, and $\chi_e^{\delta(W)} = 0$ if $e \notin \delta(W)$. This yields a $1-1$ correspondence between the cuts of $G$ and their $\{0,1\}$ incidence vectors in $\mathbb{R}^E$. The cut-polytope $P_C(G)$ of $G$ is the convex hull of all incidence vectors of cuts of $G$, i.e.

$$P_C(G) = \mathrm{conv}\{\chi^{\delta(W)} \in \mathbb{R}^E \mid W \subseteq V\}.$$

The problem of finding a cut $\delta(W)$ in $G$ with $\sum_{ij\in\delta(W)} c_{ij}$ as large as possible can be written as the linear program $\max\{c^T x \mid x \in P_C(G)\}$, since the vertices of the polytope $P_C(G)$ are exactly the incidence vectors of the cuts of $G$, and vice versa. In order to apply linear programming techniques to solve this linear program, one has to represent $P_C(G)$ as the solution set of an inequality system. Since the max-cut problem is $\mathcal{NP}$-hard, one cannot expect to find a complete system describing $P_C(G)$. But also partial systems turned out to be useful for solving max-cut problem instances. The facet structure of $P_C(G)$ for general graphs has been studied by several authors. Large classes of facet-defining inequalities are known (see, e.g. the survey [16]).

The *separation problem* consists of identifying one or more of the inequalities which are valid for all points in $P_C(G)$, yet are violated by a given point $\overline{x} \in \mathbb{R}^E$, or reporting that no such point exists.

The idea underlying our cutting plane approach is the following. We choose a system $S$ of linear inequalities whose solution set $P$ contains $P_C(G)$

and for which the separation problem can be solved in polynomial time. Moreover, $S$ must have the property that $P_C(G) = \text{conv}\{x \in P \mid x \text{ is integral}\} = \text{conv}\{x \mid x \text{ satisfies all inequalities in } S \text{ and } x \text{ is integral}\}$. Our aim is to solve $\max\{c^T x \mid x \in P\}$. If the optimum solution over $P$ is integral, it is the incidence vector of a cut and we are done.

In our case, the system $S$ is given by the *trivial inequalities*

$$0 \leq x_e \leq 1$$

for all $e \in E$ and the *cycle inequalities*

$$x(F) - x(C \setminus F) \leq |F| - 1$$

for all cycles $C \subseteq E$ and $F \subseteq C$, $|F|$ odd. These inequalities are derived from the fact that any cycle must intersect any cut in an even number of edges. If $C$ is a chordless cycle, the corresponding inequality is facet-defining for $P_C(G)$, i.e. necessary in a nonredundant linear description of $P_C(G)$. There is a polynomial time algorithm for the separation of cycle inequalities that is based on shortest paths computations [6].

The system $S$ is very large and it is impossible to write down all inequalities in polynomial time. First, we choose only cycle inequalities induced by the faces of the embedded grid graph in our separation routine. If we do not find any more violated inequalities of that type, we separate by inequalities induced by the triangles involving the node 0 corresponding to the magnetic field. An interesting observation is that we usually only need a few additional cycle inequalities.

Due to our insufficient knowledge of the inequalities that are necessary to describe $P_C(G)$ completely, and the fact that we do not have good algorithms for the identification of certain further classes of known facet-defining inequalities (the system $S$ only defines a proper relaxation of the max-cut problem), we may end up with a nonintegral solution $\overline{x}$. In this case, we branch on some fractional variable $x_e$ (i.e. a variable with $\overline{x}_e \notin \{0,1\}$), creating two subproblems in one of which $x_e$ is set to 0 and in the other $x_e$ is set to 1. Then we apply the cutting plane algorithm recursively for both subproblems. This type of method is called *branch and cut.*

An interesting point in our computational experiments is that, in most cases, the cycle inequalities turn out to be sufficient for solving the max-cut problems without branching, although we know that there are facet-defining inequalities that our algorithm does not identify. In fact, our implementation does contain simple heuristics for identifying further facet-defining inequalities whenever we cannot identify any more cycle inequalities.

## 4. Computational experiments

Our computational experiments were carried out on a SUN SPARCstation 10 and a DEC Alpha/OSF1. The complete computer code, except the linear programming routines, was written by us; to solve the linear programs we used the CPLEX Callable Library [10].

As a first experiment, we considered toroidal $L \times L$ grids with $L$ up to 100, in which the interactions $J_{ij}$ were chosen according to a Gaussian distribution with mean 0 and standard deviation 1, at zero field. For each $L$ between 5 and 50, we did $\lceil 10^5/L^2 \rceil$ runs, i.e., a total of 20 174 ground state computations. These experiments were run on a SPARCstation 10 and each of them took less than 15 minutes of CPU time. For $L = 60, 70, 80, 90, 100$, we did 20 experiments each. These experiments were run on a DEC Alpha/OSF1. Solving the $100 \times 100$ instances took between 1.5 and 8 hours, 4 hours on average. In Figure 1 we show the ground state energy versus the grid size. For each value of $L$ we show the average, the minimum, and the maximum ground state energy, taken over all samples of that size. In addition, for

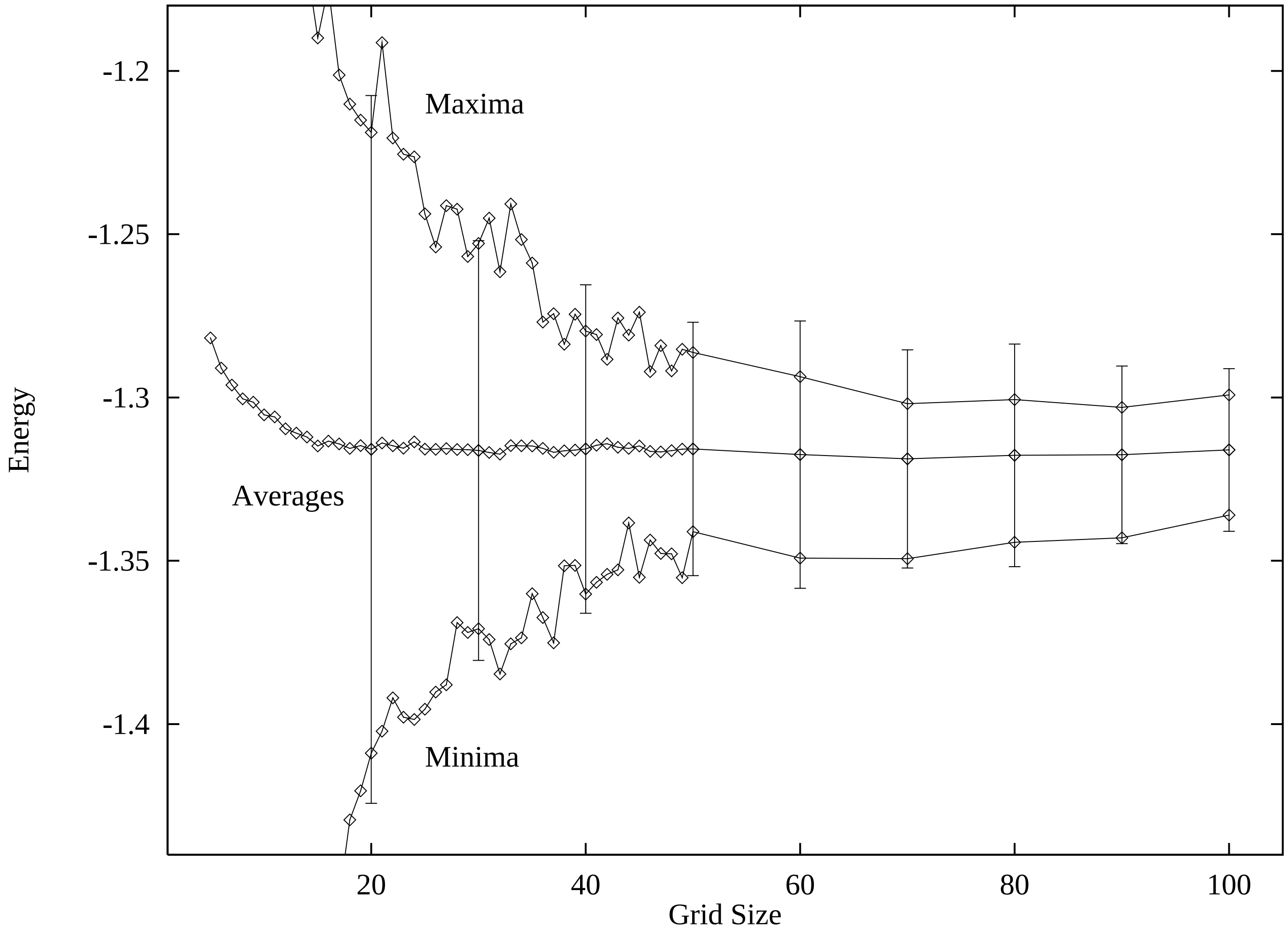


Fig. 1.  Ground state energy vs. grid size

$L = 20, 30, \ldots, 100$ a vertical bar represents the interval $\mu \pm 3\sigma$, where $\mu$ and $\sigma$ denote the average and the standard deviation, respectively.

It is an interesting question how the average ground state energy depends on the grid size (at zero magnetic field). If one can extrapolate important information (e.g., the ground state energy) from small sizes to bigger ones, we have a fast tool for finding such information. With Figure 1 we try to address this issue.

The ground state energy values for the small grids show a very high variance. We expected this behavior because of the great influence of randomness in small systems. We fit the data with an $\log(E(L) - E_0) \propto -L$ curve, where $L$ is the grid size, taking into account the average ground state energy values for $L = 20, 30, \ldots, 100$. This fit suggests a ground state energy of $E_0 = -1.3177 \pm 0.0014$. The grid sizes we can handle efficiently lie already in the asymptotic part of the fitting curve. We also fit the data with a constant value and we got the estimate $E_0 = -1.3168 \pm 0.0004$. Both fits are consistent with but more accurate than the estimate of $E_0 = -1.31 \pm 0.01$ we found in [9].

The curves given in Figure 2 show the ground state energy and the ground state magnetization as a function of the exterior magnetic field varying between 0 and 4 by 0.2. Using a similar technique as in [5] and [11], we can save a lot of time by solving such a sequence of instances in which only the field changes, instead of solving each instance from scratch. Taken alone, instances with high field are much easier for our algorithm than those with small field. For each value of the field, we ran ten $50 \times 50$ instances. Figure 2 shows the averages for ground state energy and magnetization values.

Finally, we would like to repeat the experiment by Barahona [4], namely estimating the exponent $1/\delta$ in the expression $m(F) \propto F^{1/\delta}$, for the magneti-

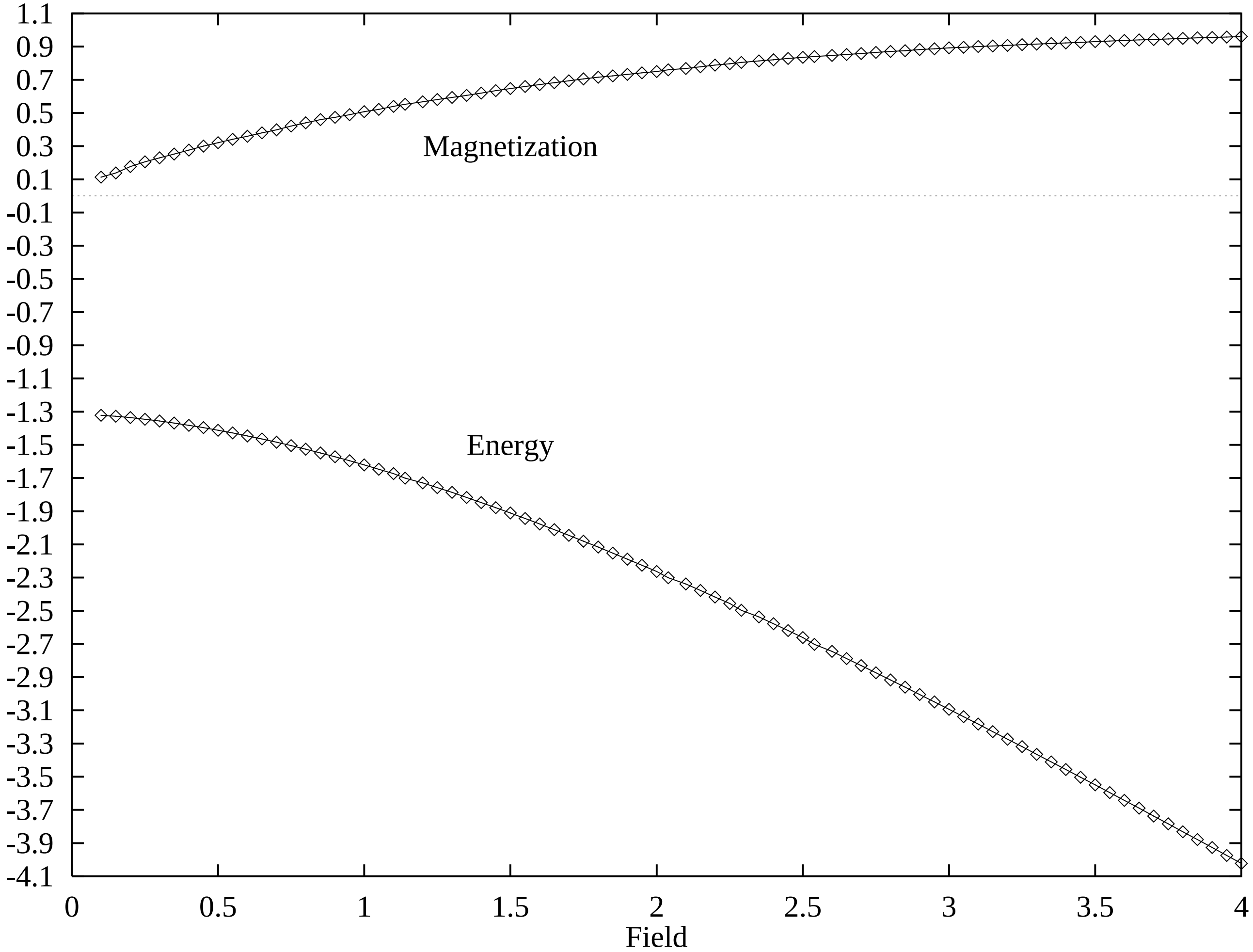


Fig. 2. Development of magnetization and energy with increasing field

zation $m$ and the field $F$. Doing the same kind of computation based on ten $50 \times 50$ grids for 20 different values of $F$ (instead of grids of sizes $25 \times 25$, $30 \times 30$, and $35 \times 35$, ten instances each, for five different values of $F$), we can give the estimate $1/\delta = 0.651 \pm 0.004$ from the fit in Figure 3, confirming Barahona's estimate of $0.648 \pm 0.038$. Barahona's estimate was already in disagreement with various other estimates in the literature, but it was still compatible with the estimate of 0.678 given in [15]. Our estimate disagrees also with this one.

## 5. Final remarks

In this paper, we investigated exact ground state computations for Ising spin glasses on 2-dimensional grids with nearest neighbor and periodic boundary interactions, based on a Gaussian bond distribution, and an exterior magnetic field. Our approach is applicable to any spin glass model in the Edwards-Anderson sense, i.e., any configuration (2- or 3-dimensional, grids with or without periodic boundary conditions, with or without magnetic field, ...) and any interaction pattern (short range or long range interactions, interaction values drawn from a Gaussian distribution, or taken as $\pm J$ with random distributions of a certain percentage of negative interactions, ...). Preliminary computational results indicate that, e.g., replacing "Gaussian" with "$\pm J$" tends to yield considerably harder problem instances for our approach. We plan to investigate this further. In addition, we plan to investigate 3-dimensional grids with various interaction patterns.

## Acknowledgement

We would like to thank Dietrich Stauffer for encouraging us to write this paper and for his help in improving its presentation.

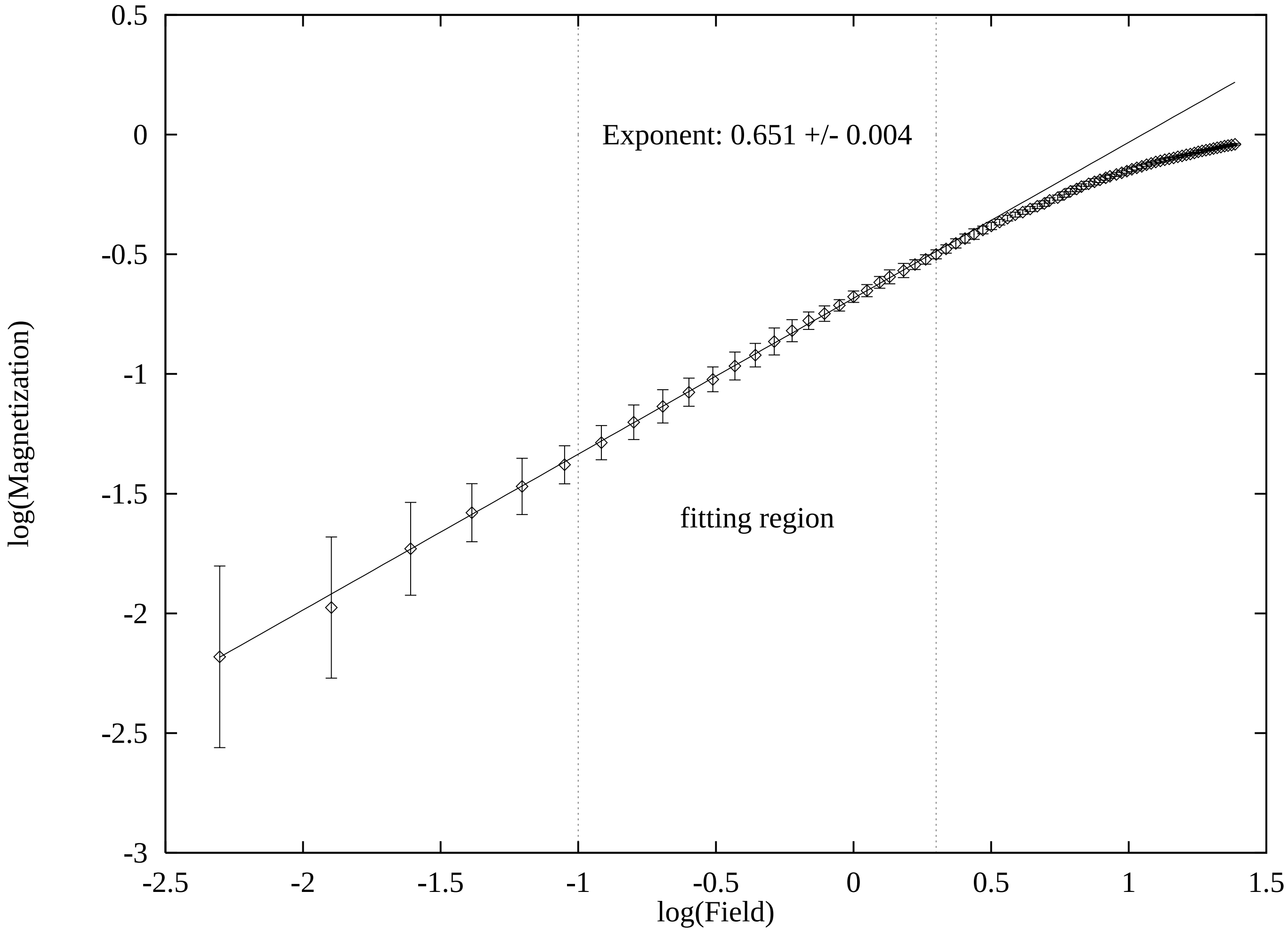


Fig. 3. Verifying a power law for the magnetization

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