Comparison of Genetic Algorithms and Particle Swarm Optimization on the Problem of Locating Ground States of Ising Spin Glasses*

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Abstract

The main objective of the research presented in this paper is to compare the overall performance of genetic algorithms (GA) and particle swarm optimization (PSO) for the problem of finding ground states for various configurations of Ising spin glasses on a grid with nearest neighbor and periodic boundary interactions, with or without the presence of exterior magnetic field. Experimental results show that the quality of PSO and GA solutions are similar, with slightly better results for PSO.

1. Introduction

One of the dominant themes in the history of physics in this century has been the effort to understand condensed states of matter. This began with very simple systems and has gradually developed to include more and more complex and subtle states and phenomena. Spin Glasses are the current frontier in this development, the most complex kind of condensed state encountered so far in solid state physics[16]. In order to present our experiments and results, some introduction to the Ising model of spin glasses, and also GA and PSO is due.

1.1. Spin glasses

Each atom that composes matter carries a spin generated by the motion of the electrons around its nucleus, which in turn generates a microscopic magnetic field around the atom. To simplify matters, assume that the spin can take only two opposite directions: up and down. At high temperature, i.e. above some material dependent critical temperature T_c, the motion of spins is so erratic that at any time about half of them are pointing up and half are pointing down, and the individual microscopic magnetic fields generated by the spins cancel each other out, resulting in zero macroscopic magnetization. In ferromagnets (materials capable of attracting pieces of iron placed in their vicinity), below the critical temperature, each spin has a tendency to align with the spins in its neighborhood, and the individual microscopic magnetic fields sum up to create a macroscopic magnetic field. By contrast, in spin glasses, only some pairs of neighboring spins prefer to be aligned, while the others prefer to be anti-aligned, resulting in two types of interactions: ferromagnetic and anti-ferromagnetic. Because of this mix of interactions these systems are called disordered [5]. Some examples of spin glasses are disordered magnetic alloys, i.e., metals containing random magnetic impurities, such as AuFe or CuMn.

1.2. The Ising Model

The Ising model was named after the German physicist Ernst Ising. In 1925, he introduced in his PhD dissertation this mathematical model for phase transitions, i.e. abrupt changes of state that occur, for example, when water freezes or a cooling lump of iron becomes magnetic. The goal of the Ising model is to explain how long-range correlations are generated by local interactions.

We will follow the presentation of the model found in [3]. The Ising model can be formulated in any dimension in graph-theoretic terms. Vertices of the graph $G = (V, E)$ represent atoms in a crystal and edges represent bonds between adjacent atoms. In the classic model, the graph is the standard "square" lattice in one, two, or three dimensions, so that each atom has two, four, or six "nearest neighbors", respectively. Each edge has assigned a coupling constant, denoted by $J_{ij} \in \{-J, J\}$, where i and j are the two vertices of the edge, and $J = 1$ usually. If we denote by S the state of the hole system, then each vertex i can be in one of two states, usually written as $S_i = \pm 1$. The interaction between neighboring vertices i and j contributes an amount $-J_{ij}S_iS_j$ to the total energy H (the Hamiltonian) of the

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system in the state S, so that

$$H(S) = -\sum_{ij \in E} J_{ij} S_i S_j. \tag{1}$$

If J_{ij} is positive, then having neighbors in the same state ($S_i = S_j$) decreases the total energy. If all the coupling constants are positive, the lowest-energy configuration of the system is with all its vertices in the same state. If the coupling constants are a mix of positive and negative numbers—as they are for the class of Ising models known as spin glasses—finding the "ground state" can be quite a frustrating experience. The most common configurations in the literature are 2-dimensional Ising spin glasses on a grid with nearest neighbor interactions. Periodic boundary conditions are often used as a way to approximate infinite size spin glasses on a finite number of spins.

In 1982, Francisco Barahona showed that finding a ground state for the three-value coupling constant ($J_{ij} \in \{-1, 0, 1\}$) on a cubic grid is equivalent to finding a maximum set of independent edges in a graph for which each vertex has degree 3. He also showed that computing the minimum value of $H(S) = -\sum_{ij} S_i S_j - \sum_i S_i$ (the hamiltonian of a spin glass with an external magnetic field) is equivalent to solving the problem of finding the largest set of disconnected vertices in a planar, degree-3 graph. Therefore Barahona uncovered that three-dimensional spin glass model for the standard square lattice, and the planar model with an external field, are NP-complete. Based on the work of Barahona, Sorin Istrail showed that the essential ingredient in the NP-completeness of the Ising model is non planarity[10].

2. Nature Inspired Approaches

2.1. Genetic Algorithms

Genetic Algorithms (GAs) are a particular class of evolutionary algorithms (EAs), introduced by John Holland [9] as a computational analogy of adaptive systems. GAs are search procedures based on the mechanics of natural selection and natural genetics. Thus, one may say that their source of inspiration is the Darwinian evolutionary theory.

GAs are implemented as a computer simulation of an environment, influenced by the optimization problem tackled, in which one or more populations of one or more species "evolve" as time passes by. Each individual (or chromosome) in these populations encodes a problem candidate solution. Through evolution, individuals try to find better suited features for their environment, thus finding better solutions to the problem. After some time individuals will "die", but their good features are likely to survive in their offspring.

The evolution starts from a population of completely random individuals and happens in generations. In each generation, individuals evolve by means of some genetic operators, they are assigned fitness values (as a measure of their adaptation to the problem), and a stochastically selection process (based on their fitness) is applied to create the population of the next iteration.

The classical representation[13] of individuals (as fixed-length binary strings of 0s and 1s), is very well suited to the purpose of this research. The state of a system with n spins can be encoded as a n-sized binary string, with the value of the i^{th} bit representing the state of the i^{th} spin: 0 for down and 1 for up.

The classical genetic operators for binary string encoding, mutation and crossover, can be used straightforward. Mutation acts on each gene (i.e. bit) by swapping its value with some very low probability (p_m), usually less than 1%. Crossover operates on two individuals by swapping parts between then, thus creating new offspring with features common to both parents. Since crossover is considered more important than mutation, its application rate is very high, usually more than 60%.

The raw fitness of some chromosome c is computed by a straightforward variation on (1)

$$rf(c) = -\sum_{1 \le i < j \le n} J_{ij}(2c_i - 1)(2c_j - 1) \tag{2}$$

where c_i is the i^{th} bit of c. In this research, lower raw fitness values indicate better solutions. The standardized fitness, used for roulette wheel selection[2], is computed by

$$sf(c) = \frac{rf(c) - min_{rf}}{\sum_{c' \in C} (rf(c') - min_{rf})} \tag{3}$$

where C denotes the current population and $min_{rf} = \min_{c' \in C} rf(c')$.

More information about research related to GAs applied for finding spin glasses ground states can be found in the literature [1] [7] [8] [14] [15] [17] [18] [19].

2.2. Particle Swarm Optimization

Particle Swarm Optimization (PSO) is a meta-heuristic inspired by the social behavior of bird flocking or fish schooling, introduced in 1995 by James Kennedy and Russel Eberhart[6]. Similar to GAs and other EAs, PSO tries to solve optimization problems using a set (called swarm) of potential solutions (called particles). Unlike GAs, PSO has no evolution operators and the particles do not compete with one another for survival; they all survive and, moreover, they share gathered information for the welfare of the swarm[4]. The function describing the problem we tackle generates a landscape in which particles improve their "quality of life" not by evolving—like GAs does, but by "flying" toward more promising areas.

The process starts with a swarm of particles randomly scattered around the search space, that move with each iteration toward more promising locations. During the flight, each particle steers, i.e. updates its speed and position, according to its own past experience and that of its most successful neighbor.

The binary decision form of the PSO[11] can be applied directly in this research. In this case, the i^{th} component of the position vector of a particle encodes the state of the i^{th} spin glass in the system (0 means down, 1 means up), while the i^{th} component of the velocity vector determine the confidence that the i^{th} spin glass should be up.

On each iteration, each particle updates its velocity and position vectors (i.e. its confidence and decision) based on the formulae

$$v'_t = v_{t-1} + \phi_1 c_1 (p_p - p_{t-1}) + \phi_2 c_2 (p_g - p_{t-1}) \quad (4)$$

$$v_t = \max(-v_{max}, \min(v_{max}, v'_t)) \quad (5)$$

$$p_t = \begin{cases} 1, & \text{if } \phi_3 < \dfrac{1}{1+\exp(-v_t)} \\ 0, & \text{otherwise} \end{cases} \quad (6)$$

where ϕ_i are random constants, p_t and p_p are the particle's current and best position, respectively, and p_g is the best position of the most successful neighbor of the particle. The parameter v_{max} limits the speed of the particle, preventing the explosion of the swarm. Usually, other parameters like the Eberhart's inertia weight or Clerc's Type 1 constriction coefficient may also be employed to produce convergence of the search.[6]. Once a particle's position is known, its profit can be computed by (2) in which c is replaced by p.

To the best of the authors' knowledge, there have been no attempts to tackle the problem of finding spin glasses ground states with the help of PSO. However many studies indicate that PSO is a worthy opponent for GAs on similar combinatorial optimization problems[12].

3. Experiments

Other papers[18] analyzed the ability of GAs to find an exact (or near-exact) ground state of a limited number of 2-dimensional and 3-dimensional $\pm J$ spin glasses, ground states that were previously found by a brute-force algorithm. To this end, large time and computational resources were allocated to GA (a run-time of over 6 weeks). Our research compares the overall performance of genetic algorithms and particle swarm optimization for the problem of finding ground states in many various scenarios randomly generated based on a some known parameters.

3.1. Setup

The setup of a GA with binary string encoding includes at least the crossover type (one-point, two-points, uniform) and rate (p_c), the mutation rate (p_m), the selection scheme (roulette wheel, tournament, ranked, with or without elitism), maximum number of generations. The setup of PSO presents a large number of choices also: individual (c_1) and social (c_2) "learning skills", maximum speed (v_{max}), inertia weight (ω), maximum number of iterations. Because of limited computational resources we used parameters for which good results were reported in the literature[6][13] for various similar problems. Hence, in all the experiments we used the same parameters presented in Tables 1 and 2. In order to reduce the computational time without decreasing the difficulty of the problems, spin glasses of up to 125 spins were considered with a very low number of individuals in GA and particles in PSO.

Parameter	**Value**
Population size	30
Crossover type	one-point cut
Crossover rate	60%
Mutation rate	1%
Selection	roulette-wheel
No. of generations	100

Table 1. GA parameters

Parameter	**Value**
No. of particles	30
Individual learning	2
Social learning	2
Inertia weight	0.9
Speed limit	0.1
Neighborhood size	2
No. of iterations	100

Table 2. PSO parameters

In the first stage of the research, we considered 1-dimensional spin glasses systems of $n \in \{5i | 1 \leq i \leq 10\}$ spins. For each size, three amplitudes J are randomly selected from $\{0.1i | 1 \leq i \leq 20\}$. For each amplitude value, a spin glass configuration is generated with random ferromagnetic or anti-ferromagnetic nearest neighbor interactions of that amplitude. For each spin glass, GA and PSO were run 30 times in a null-value external magnetic field and 30 times with an external magnetic field of magnitude -0.5, resulting in a total of 60 different test problems.

In the second stage, test problems were randomly generated based on various parameters. The main parameter is the dimensionality of the spin glass (1, 2 or 3-dimensional).

The second parameter is the size of the grid along each dimension which varies from 1 to 5, skipping some redundant or uninteresting configurations. Based on the dimensionality and size parameters, a total of 14 test cases are generated (varying from 2-dimensional 2×2 spins to 3-dimensional $5 \times 5 \times 5$ spins systems), all of them having periodic boundary conditions. For each test case, three amplitudes J are randomly selected from $\{0.1i | 1 \leq i \leq 20\}$ and three spin glass configurations are generated with random ferromagnetic or anti-ferromagnetic nearest neighbor interactions of those amplitudes. For each of the resulting spin glass, GA and PSO were run 30 times without an external magnetic field and 30 times with an external magnetic field of magnitude -0.25, resulting in a total of 84 different test problems.

3.2. Results

Tables 3 and 4 and the following figures present the average values for the number of iterations in which the best solution was found, the system energy, and the run-time for both GA and PSO on each of the test problems. Obviously, the most important result is the system energy, with lower values associated to better results. In the majority of cases, PSO outperformed GA, yet in all cases the difference was very small. The average run-times (obtained with Matlab 7 software on a PC with Pentium 4 at 2.8GHz processor) are also important results which may help to predict run-time for larger dimension spin glasses. Again PSO and GA have similar results.

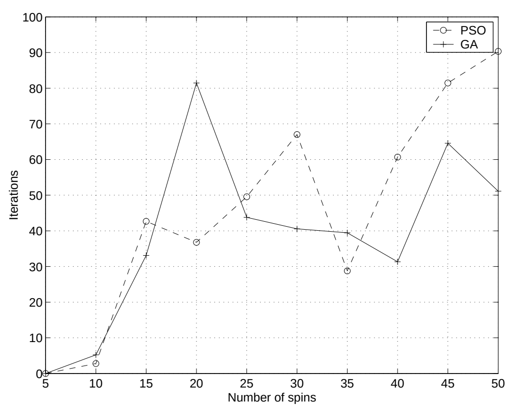

Figure 1. Average no. of iterations until a solution is found in stage 1 problems without external magnetic field

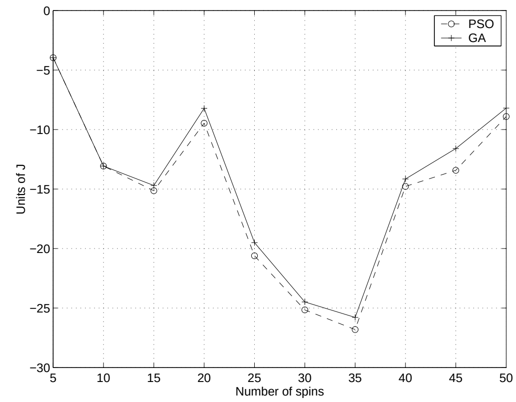

Figure 2. Average system energy in stage 1 problems without external magnetic field

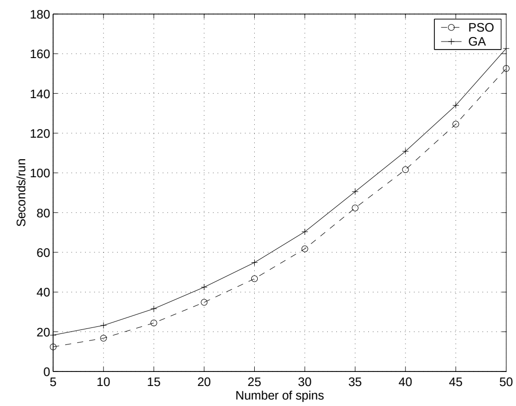

Figure 3. Average run-time in stage 1 problems without external magnetic field

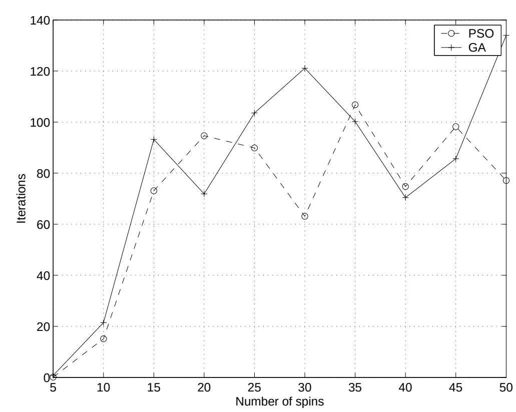

Figure 4. Average no. of iterations until a solution is found in stage 1 problems with external magnetic field

4. Conclusions

On the randomly generated test problems, both GA and PSO performed very well, with PSO outperforming GA by

Spins	With external magnetic field						Zero external magnetic field					
	Iterations		Energy		Run-time		Iterations		Energy		Run-time	
	PSO	**GA**	**PSO**	**GA**	**PSO**	**GA**	**PSO**	**GA**	**PSO**	**GA**	**PSO**	**GA**
5	0.1	0.8	-4.5	-4.5	14.4	19.2	0.0	0.0	-4.0	-4.0	12.4	18.3
10	15.1	21.4	-13.3	-13.3	19.0	24.4	2.8	5.2	-13.1	-13.1	16.8	23.2
15	73.1	93.2	-10.2	-10.2	26.4	32.5	42.7	33.1	-15.1	-14.7	24.5	31.6
20	94.7	71.9	-15.7	-15.6	36.7	43.3	36.8	81.4	-9.5	-8.2	34.8	42.5
25	89.9	103.6	-23.5	-22.6	49.2	56.4	49.6	43.8	-20.6	-19.5	46.7	54.9
30	63.1	121.1	-25.1	-25.0	64.8	72.2	67.0	40.6	-25.2	-24.5	61.7	70.4
35	106.8	100.2	-17.3	-17.2	82.8	90.6	28.8	39.4	-26.8	-25.8	82.3	90.5
40	74.8	70.4	-19.8	-19.8	103.3	111.6	60.7	31.3	-14.8	-14.2	101.6	110.9
45	98.2	85.7	-29.2	-27.4	126.6	135.2	81.4	64.6	-13.4	-11.6	124.6	134.0
50	77.1	134.0	-22.5	-21.8	152.2	161.5	90.3	51.1	-8.2	-8.9	152.6	162.6

Table 3. Stage 1 problem results

Case	Spins	With external magnetic field						Zero external magnetic field					
		Iterations		Energy		Run-time		Iterations		Energy		Run-time	
		PSO	**GA**	**PSO**	**GA**	**PSO**	**GA**	**PSO**	**GA**	**PSO**	**GA**	**PSO**	**GA**
1	$1 \times 2 \times 2$	0.1	0.0	-4.7	-4.7	3.9	3.8	0.0	0.0	-3.1	-3.1	3.7	3.7
2	$1 \times 3 \times 2$	1.6	3.4	-14.3	-14.3	4.3	4.3	0.7	0.3	-6.2	-6.2	4.2	4.3
3	$1 \times 3 \times 3$	13.2	15.3	-4.8	-4.8	5.2	5.2	5.6	3.4	-14.7	-14.7	5.2	5.4
4	$1 \times 4 \times 4$	55.0	38.1	-24.1	-23.3	9.4	9.4	32.9	27.4	-17.4	-16.1	9.0	9.1
5	$1 \times 4 \times 5$	67.2	51.6	-18.9	-18.8	12.3	13.3	57.4	38.2	-36.3	-32.4	11.4	12.1
6	$1 \times 5 \times 5$	46.0	43.8	-33.0	-31.0	16.5	16.9	22.3	27.2	-23.9	-23.1	16.4	16.7
7	$2 \times 2 \times 2$	3.4	9.8	-13.0	-13.0	4.9	4.9	1.4	8.0	-7.3	-7.3	4.6	4.7
8	$2 \times 3 \times 2$	51.3	36.2	-22.1	-21.7	6.4	6.5	6.6	11.7	-17.8	-17.1	6.1	6.2
9	$3 \times 2 \times 3$	57.4	60.2	-23.5	-21.4	11.5	12.6	36.9	36.8	-19.1	-17.1	9.5	10.0
10	$3 \times 3 \times 3$	68.4	42.4	-42.8	-40.8	22.1	22.0	35.7	45.4	-21.9	-19.4	16.4	17.8
11	$2 \times 4 \times 4$	30.4	56.6	-41.2	-39.3	25.0	25.8	32.9	52.6	-37.7	-36.0	23.7	24.4
12	$2 \times 4 \times 5$	33.8	58.8	-24.8	-23.4	35.9	37.5	63.0	44.4	-48.2	-44.7	33.9	35.1
13	$2 \times 5 \times 5$	29.1	61.8	-39.2	-36.9	54.9	56.9	50.6	42.1	-21.5	-20.3	51.0	52.4
14	$5 \times 5 \times 5$	65.4	39.9	-125.8	-118.2	265.2	270.7	45.9	46.3	-95.6	-90.8	266.2	270.7

Table 4. Stage 2 problems results

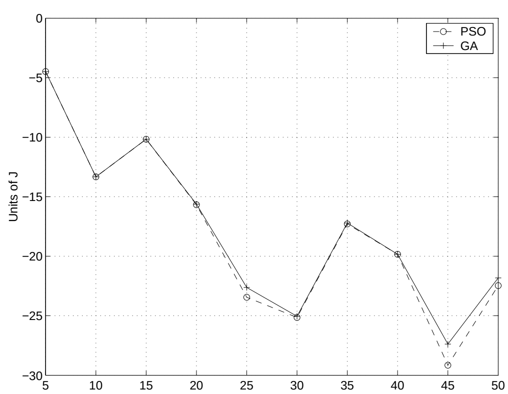

Figure 5. Average system energy in stage 1 problems with external magnetic field

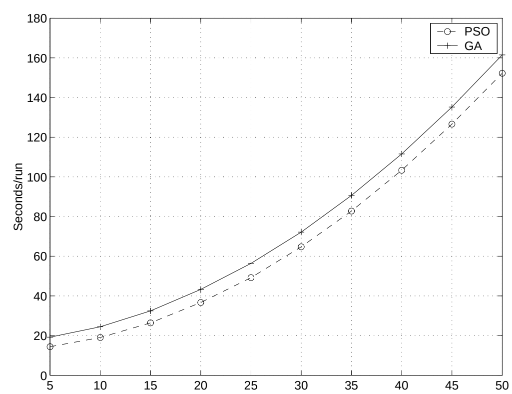

Figure 6. Average run-time in stage 1 problems with external magnetic field

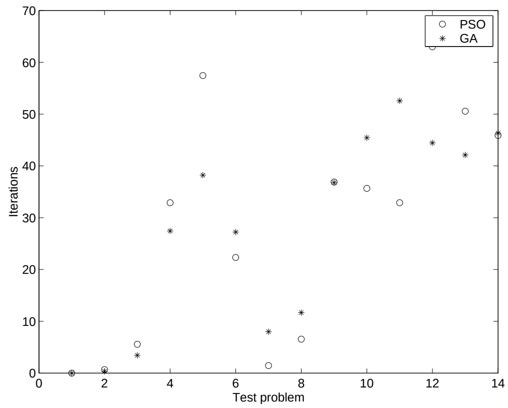

Figure 7. Average no. of iterations until a solution is found in stage 2 problems without external magnetic field

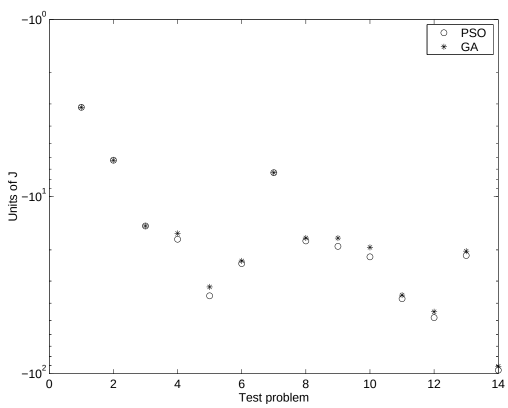

Figure 8. Average system energy in stage 2 problems without external magnetic field

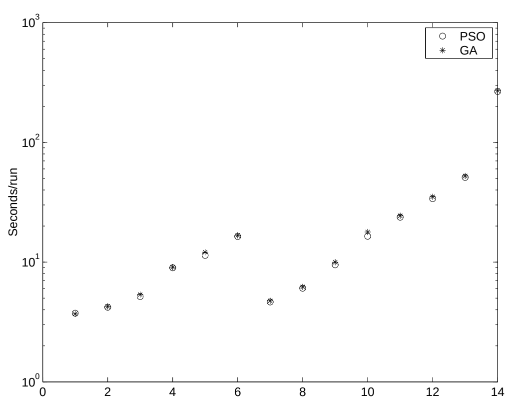

Figure 9. Average run-time in stage 2 problems without external magnetic field

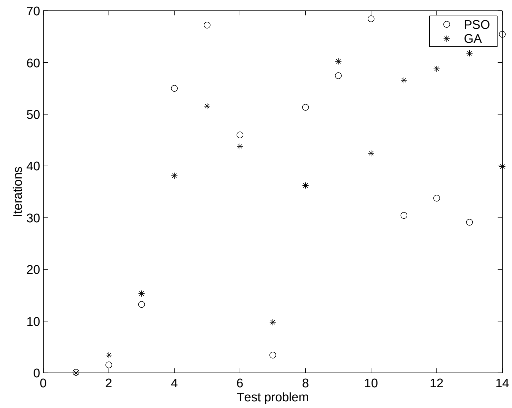

Figure 10. Average no. of iterations until a solution is found in stage 2 problems with external magnetic field

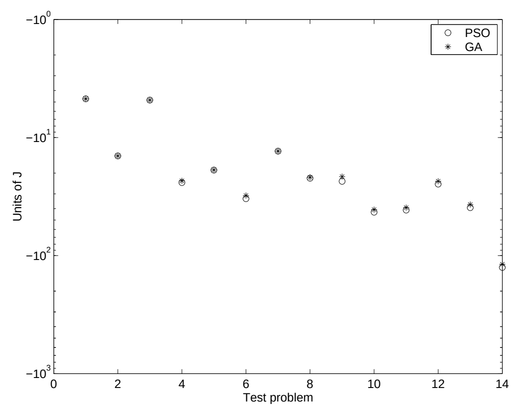

Figure 11. Average system energy in stage 2 problems with external magnetic field

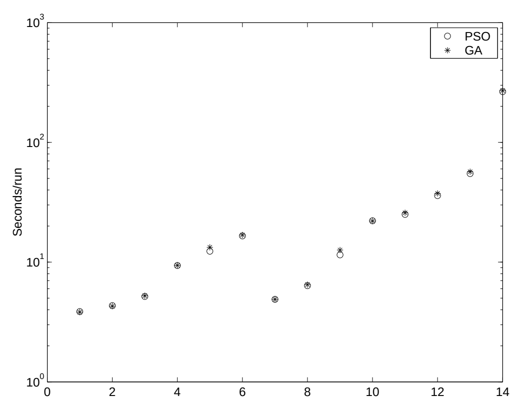

Figure 12. Average run-time in stage 2 problems with external magnetic field

a small amount. The main advantage of using these methods for this type of optimization problems is the lack of constraints regarding the dimensionality of the problem, i.e. these methods can be extended to higher dimensional systems with little effort. Hence, GAs and PSO proved to be useful tools in spin glasses research and related problems in statistical physics.

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