A general learning algorithm for solving optimization problems and its application to the spin glass problem

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We propose a general learning algorithm for solving optimization problems, based on a simple strategy of trial and adaptation. The algorithm maintains a probability distribution of possible solutions (configurations), which is updated continuously in the learning process. As the probability distribution evolves, better and better solutions are shown to emerge. The performance of the algorithm is illustrated by the application to the problem of finding the ground state of the Ising spin glass. A simple theoretical understanding of the algorithm is also presented.

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Many problems in science and engineering can be formulated in terms of optimization problems. In these problems we often want to find a set of optimum values for a set of variables that minimizes a given function of the variables. When the number of variables is large, especially in cases where there are a number of local minima, an exact solution is usually impossible to obtain; the aim is thus to find near-optimal solutions.

A few optimization methods, based on ideas from physics and biology, have been developed recently which lead to rather good general purpose algorithms \[1\] for solving optimization problems. They have been successfully applied to a wide range of practical problems. One of them is a stochastic algorithm known as optimization by simulated annealing (OSA) \[2\]. The method is based on an analogy with thermodynamics, in particular, on the way in which the atoms in a liquid find their minimum energy configuration of a crystal, when the liquid is annealed or cooled slowly. The algorithm consists of Monte Carlo dynamics performed at a sequence of effective temperatures to simulate the effect of annealing. The stochastic dynamics allows access to a larger region of configuration (solution) space than simple “quenching” methods, and thereby helps in reaching a good solution. However, the Monte Carlo search is based on evolution of a single starting configuration and is thus often confined to a limited region of configuration space and is consequently not efficient in searching through configuration space. Many ideas have been proposed to make OSA efficient. For example, the OSA based on the multi-canonical sampling technique has proved quite effective in the spin glass problem \[3\] and the traveling salesman problem \[6\]. Another general purpose algorithm which has been used extensively is the Genetic Algorithm (GA) \[3\]. The Genetic Algorithm demonstrates the importance of keeping many configurations (“species”) in the optimization process. The algorithm mimics the principles of evolution (using crossover, mutation, etc. to update the configurations). GAs have been applied to a large range of problems in a wide variety of topics. To apply GAs to large-size problems, however, a significant number of configurations need to be retained (thus imposing memory requirements) and in addition, many independent runs may be needed to avoid missing out on good solutions. Thus GAs may not be efficient for optimizing large-size problems.

In this paper, we propose a learning algorithm, which is as general as the genetic algorithm, but does not require storing many configurations explicitly. What is kept and updated in our learning algorithm are probability weights associated with each spin that enable one to generate new configurations probabilistically, with lower energy configurations favored; this allows many configurations to be kept implicitly. The learning process is constructed in such way that the evolution of the probability distribution will lead to better and better configurations (solutions). An early version of the algorithm has been applied to solve the traveling salesman problem \[7\]. We first present the general algorithm and demonstrate analytically that in its simplest version the algorithm leads to progressively more optimal solutions. In the second part of the paper we present explicit results for the problem of determining the ground state of the Ising spin glass.

To describe the algorithm, let us consider the general optimization problem of finding the values of a set of variables or parameters \(\{\lambda_i, \ i = 1, 2, \ldots, n\}\) such that the function \(F(\lambda_1, \lambda_2, \ldots, \lambda_n)\) is a minimum; \(F\) represents a (free) energy or an objective function. As is done in GAs, we encode the variables \(\lambda_i\) using binary digits, and write the function as \(F(\sigma_1, \sigma_2, \ldots, \sigma_N)\), where \(\{\sigma_k, \ k = 1, 2, \ldots, N\}\) are binary numbers assuming values 0 and 1. Equivalently, we may use spin variables \(s_i\) with values -1 and 1. Since we will test our algorithm on the spin glass problem, we will employ the spin description from now on.

The aim of the optimization is to find the spin configuration \(\{s_i\}\) that gives rise to the smallest value of \(F\). The learning algorithm for this problem can be formulated as follows. For each spin \(s_i\), a weight \(w_i\) is assigned. The probability for choosing \(s_i = 1\) is defined as \(w_i/(1 + w_i)\) and the probability for choosing \(s_i = -1\) is then \(1/(1 + w_i)\) (Initially \(w_i\) is set to be 1, so that the probabilities of choosing \(s_i = 1\) and \(s_i = -1\) are equal). The basic ingredients in the algorithm are trial and adaptation: first select a configuration \(\{s_i\}\); then modify the weights \(\{w_i\}\) to favor configurations with smaller values of \(F\).

Selection of Spin Configuration: A configuration is selected by choosing the initial configuration \(\{s_i\}\) with the probability determined by the weights \(\{w_i\}\). In the simplest version of the algorithm, this configuration is used in the evaluation for updating the weights. The performance of the algorithm can be greatly improved by implementing a local optimization on the configuration (changing \(s_i\) from 1 to -1 and vice versa). The resulting configuration after the local optimization will then be used for the updating (evaluation) of the weights. The simplest way to perform the local optimization, which is quite general, consists of individual spin flips to lower the value of \(F\). More sophisticated algorithms can also be used. But they are likely to be problem dependent.

Evaluation of the configurations obtained and modification of weights: Starting from the second trial, the configuration obtained in the current trial is compared with the configuration obtained in the previous trial. Let \(\{s_1, s_2, \ldots\}\) denote the current configuration and \(\{s'_1, s'_2, \ldots\}\) denote the previous configuration; let the corresponding values of the function to be minimized be \(F\) and \(F'\) respectively. The comparison of these two configurations leads to the modification of weights described by the equation:

\[
  w_i^{\text{new}} = w_i^{\text{old}} e^{-\alpha(F-F')(s_i-s'_i)/2}, \quad i = 1, \ldots, N, \tag{1}
\]

where \(N\) is the total number of spins in the systems, and \(\alpha\) represents the modification rate of weights (learning rate
of the algorithm). According to this rule, if the functional value of the current configuration, $F$, is lower (higher) than the previous one, $F'$, the weight will be modified to favor (disfavor) the current spin configuration. The new weights will be used in the selection of the next configuration according to the prescription given earlier and the procedure repeated. As learning advances, the spin configuration will be gradually “frozen” into a near-optimal configuration.

We study the simplest version of the model analytically to understand how the learning process leads to better solutions. We consider the limit where the learning rate $\alpha$ is very small, and consequently $w_i$ changes very slowly. In the spirit of the “adiabatic approximation” we can write down an equation describing the change of the weight as a function of time (defined as the number of trials used):

$$\frac{dw_i}{dt} = \left[ \sum_{s_1, \ldots, s_N} \sum_{s'_1, \ldots, s'_n} P(s_1, \ldots, s_N)P(s'_1, \ldots, s'_n) \left( e^{-\alpha(F(s_1, \ldots, s_N) - F(s'_1, \ldots, s'_n))(s_i - s'_i)/2} - 1 \right) \right] w_i, \quad (2)$$

where $P(s_1, \ldots, s_N)$ is the probability of generating the configuration $\{s_1, \ldots, s_N\}$. Since each spin is chosen independently, the probability $P$ can be written as

$$P(s_1, s_2, \ldots, s_N) = \prod_i p(s_i),$$

where $p(s_i)$ is the probability that the $i$th spin in the configuration assumes the value $s_i$. As we have described earlier, $p(s_i)$ is given by $w_i/(1 + w_i)$ if $s_i = 1$ and $1/(1 + w_i)$ if $s_i = -1$. These can be combined into a single expression as follows:

$$p(s_i) = \frac{(1 + s_i)w_i/2 + (1 - s_i)/2}{1 + w_i} = \frac{1}{2} + s_i \frac{w_i - 1}{2w_i + 1}.$$

In the limit $\alpha \to 0$ we can expand the exponential function in the above equation and keep only the leading order term. We have

$$\frac{dw_i}{dt} = -\alpha w_i \left[ \sum_{s_1, \ldots, s_N} \sum_{s'_1, \ldots, s'_n} P(s_1, \ldots, s_N)P(s'_1, \ldots, s'_n)(F(s_1, \ldots, s_N) - F(s'_1, \ldots, s'_n))(s_i - s'_i) \right]. \quad (3)$$

Straightforward manipulations lead to

$$\frac{dw_i}{dt} = -\alpha w_i \sum_{s_1, \ldots, s_N} P(s_1, \ldots, s_N)F(s_1, \ldots, s_N)(s_i - \frac{w_i - 1}{w_i + 1}). \quad (4)$$

Given the expression for $\frac{dw_i}{dt}$, we can then evaluate the change in the average functional value as a function of time. The average is defined as

$$\bar{F} = \sum_{\{s_i\}} F(\{s_i\})P(s_1, \ldots, s_N),$$

and $\frac{d\bar{F}}{dt}$ is given by

$$\frac{d\bar{F}}{dt} = \sum_{i} \sum_{s_1, \ldots, s_N} F(s_1, \ldots, s_N)P(s_1, \ldots, s_N) \frac{1}{p(s_i)} \frac{dp(s_i)}{dt}. \quad (5)$$

Now using the fact that

$$\frac{1}{p(s_i)} \frac{dp(s_i)}{dt} = \frac{s_i}{p(s_i)} \frac{1}{(1 + w_i)^2} \frac{dw_i}{dt} = \frac{1}{2w_i} \left( \frac{w_i - 1}{w_i + 1} \right) \frac{dw_i}{dt},$$

we obtain

$$\frac{d\bar{F}}{dt} = -\frac{\alpha}{2} \sum_i \left[ \sum_{s_1, \ldots, s_N} P(s_1, \ldots, s_N)F(s_1, \ldots, s_N)(s_i - \frac{w_i - 1}{w_i + 1}) \right]^2. \quad (6)$$
It can be seen from the above equation that $\bar{F}$ in the learning process is gradually reduced ($\frac{d\bar{F}}{dt} < 0$), and thus better and better configurations are obtained as learning advances. The reduction is diminished when the learning process converges, i.e., when the probability of $s_i = 1$ approaches one ($w_i$ approaches $\infty$) or zero ($w_i$ approaches 0); in these limits $s_i = \frac{w_i - 1}{w_i + 1}$ and $\frac{d\bar{F}}{dt} = 0$. This result provides some theoretical basis for our learning algorithm, which is quite valuable as analytical understanding of optimization algorithms is typically difficult to obtain.

We illustrate the performance of the learning algorithm in the case of the Ising spin glass systems described by the Edwards-Anderson Hamiltonian

$$E = - \sum_{<ij>} J_{ij} s_i s_j,$$

where the sum includes only the nearest neighbors (4 for two-dimensional systems and 6 for three-dimensional systems); the exchange interactions $J_{ij}$, between the spins $s_i = \pm 1$, are independent quenched random variables which assume the values $\pm 1$ with equal probability. Clearly the optimization method can be used for other distributions of $J_{ij}$. The aim of the optimization is to find the spin configuration $\{s_i\}$ with the lowest value of $E$ for a given set of $J_{ij}$, or the total energy per site $e$ (defined as $E$ divided by the total number of spins in the system). The problem at hand then is to optimize $e(s_1, s_2, ..., s_N)$.

Our studies on the spin glass problems were done using a 200MHz SGI Power Challenge and a cluster of SGI Indigo workstations. The CPU times quoted in this paper have all been converted to the equivalent CPU times of the SGI Power Challenge. We have studied two-dimensional systems of size ranging from $5 \times 5$ up to $200 \times 200$ and three dimensional systems of size $4 \times 4 \times 4$ up to $25 \times 25 \times 25$. Let us first look at the performance of the simplest version of the algorithm without local optimization. Here we focus on a sample of size $20 \times 20$. The learning rate is taken to be $\alpha = 0.1$. Figure 1 shows the energy obtained vs. the CPU time $t$ spent (the data are taken every 800 iterations). It also shows the lowest energy obtained up to time $t$. These data clearly show the convergence of the learning algorithm as described in our analysis above. The simple version of the algorithm is certainly not efficient as should be expected, but the result obtained is still quite impressive in view of the simplicity of the algorithm (it reduces the energy from around 0 to about $-1.2$). Better results can be obtained using a smaller learning rate $\alpha$, but this will be more time consuming.

The simplest version of the algorithm can be improved dramatically even with a simple local optimization where single spin flips are attempted to lower the energy after the configuration is selected. In this local optimization we make a few passes through the lattice and a spin is flipped if the flipping leads to a lower energy configuration; the procedure stops when the configuration can not be improved further by flipping any individual spin on the lattice. The locally optimized configuration is then used for comparison with the previous configuration (also locally optimized). It should be mentioned that this simple local optimization technique does not utilize any special feature of the spin glass problem; it can thus also be easily applied to other optimization problems. Figure 2 shows the lowest energy obtained vs. the CPU time spent using this technique (the same $20 \times 20$ sample is used). For comparison we use four different learning rates: $\alpha = 0.1$, $\alpha = 0.5$, $\alpha = 2.5$, and $\alpha = 12.5$. It is clear that with the use of the single spin flips, the algorithm is made much more efficient. The dependence of the algorithm on the learning rate is also clearly illustrated in the graph. With large $\alpha$, the learning process converges quickly, but the result obtained is worse than the result obtained using a slower learning process. There is a tradeoff between obtaining a quick solution or a good solution, which is controlled entirely by the choice of the appropriate value of $\alpha$ in the algorithm.

In addition to the simple local optimization based on single spin flips, we can incorporate more sophisticated local optimization techniques in the algorithm. The use of sophisticated local optimization techniques is likely to be problem dependent. For the spin glass problem, we use a local optimization technique similar to the Kernighan-Lin variable-depth search algorithm used in the graph-partitioning problem and the traveling salesman problem. The idea is to replace the search for one favorable spin flip by a search for a favorable sequence of spin flips, using the energy of system to guide the search. A sequence of spin flips in the variable-depth search is obtained sequentially as follows. We start with the spin flip at a selected location in the system and search its neighbors to find the most favorable spin flip as the next spin flip in the sequence (the most favorable spin flip is one that gives rise to the lowest energy among all spin flips considered). In general, after the $k$th spin flip the neighbors of all the spins which have been flipped will be searched to find the most favorable spin flip as the $(k + 1)$st spin flip of the sequence (the flipped spins in the first $k$ spin flips of the sequence will not be considered again).

Let $\Delta E(k)$ denote the total accumulated change in energy from the energy of the starting configuration due to the $k$ spin flips. To cut short the search that most likely will not lead to a better configuration, we apply the stopping condition: the search will stop at the $k$th step if $\Delta E(k + 1)$ is greater than $2d - 2$ ($d$ is the spatial dimension). We also set a maximum number of spin flips allowed, denoted by $n$. So the search will stop when $k = n$. After the search is completed, we choose $k_0$ corresponding to the minimum $\Delta E$. If $\Delta E(k_0) < 0$, then we move the starting configuration to the energetically better configuration corresponding to $k = k_0$ (by adopting the first $k_0$ spin flips); otherwise we...
abandon all the spin flips generated in the search and keep the original configuration. A new search will be initiated starting from a new location in the system.

The implementation of the local optimization based on the variable-depth search is accomplished by keeping a linked list of starting locations for the search. This is initialized to include all lattice sites at the beginning. The starting location of the search is taken and removed from the top of the list. If a better configuration is obtained in the search, the locations of all flipped spins together with their neighbors will be appended to the list (if they are not already in the list). The local optimization will end, if the linked list is empty.

Fig. 3 shows the optimization results based on $n = 0$ (no local optimization), $n = 1$ (single spin flips are used), $n = 9$ and $n = 100$ (variable-depth search). The same $20 \times 20$ sample was used. The same learning rate $\alpha = 2.5$ is used in all the optimizations. It is clear that better local optimization leads to better overall results for the learning algorithm. For $n = 9$ and $n = 100$ the results based on local optimization alone are already quite close the optimal value (due to smaller system size), so the improvement due to the learning process is small. However for the larger systems the improvement due to the learning process can be significant. One advantage of our learning algorithm is that any local optimization technique can be incorporated easily into the algorithm. The performance of the local optimization is not sensitive to the choice of $n$ as long as $n$ is not much less than 10. In fact many searches are stopped after the first few steps because of the stopping condition we employ. The time taken to perform a local optimization with $n = 100$ is typically 10 to 15 times longer than the time required for a local optimization with only single spin flips.

The overall performance of the algorithm is summarized in Table I (for 2D systems) and Table II (for 3D systems). The number of samples we use for each system size ranges from 320 for the smallest system to 10 for the largest system. The average energy (per site) we obtained and the average time taken to reach the lowest energy configuration are listed, together with the average number of iterations used. In obtaining the results presented in the tables, local optimization with $n = 100$ (for 2D systems) and $n = 125$ (for 3D systems) was used in the learning algorithms. To compare with the results obtained in the literature, we take our best results obtained with $\alpha = 0.1$, and fit our data using the form $e_L = e_\infty + cL^{-d}$ to obtain the energy of the infinite system. The results are $e_\infty = -1.4028 \pm 0.0019$ for 2D systems and $e_\infty = -1.7857 \pm 0.0026$ for 3D systems. These are consistent with the best results quoted in the literature [12]-[16]. In particular, for two-dimensional systems, Simone et al. [12] use an exact algorithm based on the branch and cut technique to find the ground states of spin glass systems with system size up to 50 $\times$ 50. They obtain the extrapolated result $e_\infty = -1.4022 \pm 0.0003$ using the same form of the fitting function. It is not clear, however, whether their technique can be efficiently implemented for 3D systems or not (Finding the ground state of the 3D spin glass is an NP-complete problem). For 3D systems, the most efficient algorithm appears to be the one using a hybrid of Genetic Algorithm and local optimization. Pál [13] used the hybrid algorithm to study 3D systems of sizes up to $14 \times 14 \times 14$ and he obtained $e_\infty = -1.785708 \pm 0.000075$ based on the same form of the fitting function we used. Our 3D result agrees well with his result.

Our algorithm is quite fast compared with most other algorithms. For example, for $14 \times 14 \times 14$ systems, our algorithm needs, on average, 1270 seconds with $\alpha = 0.5$ to obtain the average energy of $-1.7865$. In comparison, the optimization using the hybrid GA implemented by Pál, which itself is much faster than the original genetic algorithm approach used by Sutton et al., takes, on average, 23540 seconds per run (30 runs were used) on a 134 MHz SGI Indy computer (which is about four times slower the computer we use), to get the same average energy of $-1.7865$. If we do not need especially high accuracy, we can choose a larger learning rate and obtain the result much more quickly. With $\alpha = 12.5$ we can obtain the average energy of $-1.7836$ in the average CPU time of 53.6 seconds. We can study systems of size up to $200 \times 200$ and $25 \times 25 \times 25$ with $\alpha = 12.5$ rather easily without sacrificing much accuracy.

In conclusion, we have demonstrated how a complex optimization problem can be solved by a simple learning strategy of trial and adaptation. The learning process is somewhat similar to the evolution process in Genetic Algorithms. As in GA this algorithm has the advantage that it is based on global searches in configuration space. But instead of keeping many configurations explicitly as in GAs we use probability weights to generate configurations probabilistically. Thus many configurations are implicitly kept for effective mutation and crossover through the updating of the probability weights. For the simple version of the algorithm without local optimization, we have shown analytically that the algorithm does lead to better and better solutions. Local optimization techniques can also be easily incorporated in the algorithm, which leads to a rather effective optimization method, as we have demonstrated in the spin glass problem. We believe that our learning algorithm can be equally effective in other optimization problems, in particular the ones where sophisticated local search algorithms have not been found.

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Figure captions.

Figure 1. Energy per site $e$ vs. the CPU time $t$ used for the optimization of a $20 \times 20$ systems. The filled-circle represents the energy obtained at the current time; while the filled square represents the lowest energy obtained up to time $t$. The data are taken every 800 iterations, and the optimization is performed with $\alpha = 0.1$.

Figure 2. The lowest energy obtained vs. the CPU time used, for the optimizations with $\alpha = 0.1, 0.5, 2.5$ and $12.5$. Local optimization with single spin flips are used in the algorithm.

Figure 3. The lowest energy obtained vs. the CPU time used, for the optimizations with $n = 0, n = 1, n = 9$, and $n = 100$. The learning rate for these optimizations is chosen to be $\alpha = 2.5$. The same $20 \times 20$ sample is used.

Table captions.

Table I. Average lowest energy, the CPU time, and the number of trials needed (number in parentheses) to reach the lowest energy configuration from the optimizations of the two dimensional systems of size $L \times L$ with $L = 5, 10, 20, 30, 40, 50$, and $200$. The values of the learning rate $\alpha$ used are $0.1, 0.5, 2.5$, and $12.5$. The number of samples $N_s$ used is also listed (in parentheses under the system size).

Table II. Average lowest energy, the CPU time, and number of trials needed (number in parentheses) to reach the lowest energy configuration from the optimizations of the three dimensional systems of size $L \times L \times L$ with $L = 4, 6, 8, 10, 12, 14$, and $25$. The values of the learning rate $\alpha$ used are $0.1, 0.5, 2.5$, and $12.5$. The number of samples $N_s$ used is also listed (in parentheses under the system size).
Table I

| L (N_s) | α = 0.1               | α = 0.5               | α = 2.5               | α = 12.5              |
|---------|-----------------------|-----------------------|-----------------------|-----------------------|
| 5       | -1.3405 ± 0.0051      | -1.3405 ± 0.0051      | -1.3405 ± 0.0051      | -1.3405 ± 0.0051      |
| (320)   | 0.0008 (1.0)          | 0.0008 (1.0)          | 0.0008 (1.0)          | 0.0008 (1.0)          |
| 10      | -1.3882 ± 0.0037      | -1.3882 ± 0.0037      | -1.3882 ± 0.0037      | -1.3882 ± 0.0037      |
| (160)   | 0.005 (1.8)           | 0.004 (1.7)           | 0.005 (1.8)           | 0.004 (1.7)           |
| 20      | -1.4019 ± 0.0022      | -1.4019 ± 0.0022      | -1.4018 ± 0.0022      | -1.4008 ± 0.0022      |
| (80)    | 0.74 (55)             | 0.64 (48)             | 0.46 (35)             | 0.23 (20)             |
| 30      | -1.4007 ± 0.0022      | -1.4003 ± 0.0022      | -1.3999 ± 0.0022      | -1.3984 ± 0.0023      |
| (40)    | 185 (6112)            | 51 (1747)             | 11 (389)              | 2.2 (82)              |
| 40      | -1.4001 ± 0.0024      | -1.4003 ± 0.0026      | -1.3995 ± 0.0026      | -1.3983 ± 0.0026      |
| (20)    | 1587 (28670)          | 287 (5590)            | 49 (955)              | 11 (246)              |
| 50      | -1.4002 ± 0.0030      | -1.3999 ± 0.0030      | -1.3994 ± 0.0030      | -1.3988 ± 0.0030      |
| (10)    | 4503 (53038)          | 2959 (9393)           | 547 (1883)            | 150 (579)             |
| 200     | 17259 (16893)         | -1.3976 ± 0.0005      |                      |                      |
| (10)    |                       |                        |                      |                      |
Table II

| $L(N_s)$ | $\alpha = 0.1$ | $\alpha = 0.5$ | $\alpha = 2.5$ | $\alpha = 12.5$ |
|----------|----------------|----------------|----------------|----------------|
| 4 (320)  | $-1.7453 \pm 0.0067$ | $-1.7453 \pm 0.0067$ | $-1.7453 \pm 0.0067$ | $-1.7453 \pm 0.0067$ |
| 6 (160)  | $-1.7720 \pm 0.0028$ | $-1.7721 \pm 0.0027$ | $-1.7721 \pm 0.0027$ | $-1.7714 \pm 0.0028$ |
| 8 (80)   | $-1.7855 \pm 0.0029$ | $-1.7855 \pm 0.0029$ | $-1.7849 \pm 0.0029$ | $-1.7827 \pm 0.0030$ |
| 10 (40)  | $-1.7816 \pm 0.0021$ | $-1.7811 \pm 0.0021$ | $-1.7803 \pm 0.0022$ | $-1.7771 \pm 0.0021$ |
| 12 (20)  | $-1.7816 \pm 0.0020$ | $-1.7813 \pm 0.0020$ | $-1.7800 \pm 0.0024$ | $-1.7780 \pm 0.0024$ |
| 14 (10)  | $-1.7874 \pm 0.0020$ | $-1.7865 \pm 0.0020$ | $-1.7871 \pm 0.0023$ | $-1.7836 \pm 0.0017$ |
| 25 (10)  | $-1.7815 \pm 0.0009$ |                    |                |                |
Fig. 1
Fig. 2
Fig. 3