Renormalization for Discrete Optimization

J. Houdayer and O.C. Martin

Laboratoire de Physique Théorique et Modèles Statistiques, bâtiment 100, Université Paris-Sud, F–91405 Orsay, France (Received 26 January 1999)

The renormalization group has proven to be a very powerful tool in physics for treating systems with many length scales. Here we show how it can be adapted to provide a new class of algorithms for discrete optimization. The heart of our method uses renormalization and recursion, and these processes are embedded in a genetic algorithm. The system is self-consistently optimized on all scales, leading to a high probability of finding the ground state configuration. To demonstrate the generality of such an approach, we perform tests on traveling salesman and spin glass problems. The results show that our "genetic renormalization algorithm" is extremely powerful.

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The study of disordered systems is an active and challenging subject [1], and in many cases some of the most basic consequences of randomness remain subject to controversy. Given that numerical calculations of ground state properties can shed light on these issues, it is not surprising that more and more such calculations are being performed [2]. Our goal here is to introduce and test a new general purpose approach for finding ground states in disordered and frustrated systems. In this Letter we illustrate its use on the traveling salesman problem and on the spin glass problem, showing that the ground states are found with a high probability. More generally, our novel approach should be very useful for many classes of discrete optimization problems and is thus of major interdisciplinary interest.

Although it is often claimed that physical insight into disordered systems should lead to improved optimization algorithms, thus far, there has been very little substance to uphold this view. Aside from simulated annealing [3] and generalizations thereof [4], physics inspired ideas, ranging from replica symmetry breaking to energy landscapes, have had little impact on practical algorithmic developments in optimization. Nevertheless, several ideas from physics seemed promising, including renormalization [5] and hierarchical constructions [6]. Perhaps, the impact of these attempts has been minor because the resulting algorithms were not sufficiently powerful to be competitive with the state of the art. In our work, we have found that by carefully combining some of these ideas, namely renormalization and recursion, and by embedding them in a genetic algorithm approach, highly effective algorithms could be achieved. We thus believe that the essence of the renormalization group can be fruitfully applied to discrete optimization, and we expect the use of this type of algorithm to become widespread in the near future.

Let us begin by sketching some of the standard approaches for tackling hard discrete optimization problems [7]. For such problems, it is believed that there are no fast algorithms for finding the optimum, so much effort has concentrated on the goal of quickly obtaining "good"

near-optimum solutions by heuristic means. One of the simplest heuristic algorithms is local search [8] in which a few variables are changed at a time in the search for lower energy configurations. This heuristic and numerous generalizations thereof such as simulated annealing [3] optimize very effectively on small scales, that is on scales involving a small number of variables, but break down for the larger scales that require the modification of many variables simultaneously. To tackle these large scales directly, genetic algorithms [9] use a "crossing" procedure which takes two good configurations (parents) and generates a child which combines large parts of its parents. A population of configurations is evolved from one generation to the next using these crossings followed by a selection of the best children. Unfortunately, this approach does not work well in practice because it is very difficult to take two good parents and cross them to make a child which is as good as them. This is the major bottleneck of genetic algorithms and is responsible for their limited use. For an optimization scheme to overcome these difficulties, it must explicitly treat all the scales in the problem simultaneously, the different scales being tightly coupled. To implement such a treatment, we rely on ideas from the renormalization group, the physicist's favorite tool for treating problems with many scales [10]. Our approach is based on embedding renormalization and recursion within a genetic algorithm, leading to what we call a "genetic renormalization algorithm" (GRA). To best understand the working of this approach, we now show how we have implemented it in two specific cases, the traveling salesman and the spin glass problems.

The traveling salesman problem (TSP). — This routing problem is motivated by applications in the telecommunication and transportation industries. Given N cities and their mutual distances, one is to find the shortest closed path (tour) visiting each of the cities exactly once [7]. In genetic algorithms, one takes two parents (good tours) from a population and finds the subpaths they have in common. Then a child is built by reconnecting those subpaths, either randomly or by using parts belonging to the parents if possible; ultimately, these connections are not very good and lead to a child which is less fit than its parents.

In our approach, instead of creating children as described, we engineer new configurations from subpaths that are frequently shared in the population. In practice we pick k "parents" at random and determine their common subpaths: these form the patterns which we select before engineering the child. Then we wish to find the very best child which is compatible with these patterns. (This child should thus be at least as good as its best parent.) For this new problem, each subpath is replaced by its two end cities and one bond which connects them; together with the cities which do not belong to any of the patterns, this defines a new "renormalized" TSP with fewer cities. Note that in this new TSP, we have removed all the cities inside the selected subpaths, and have "frozen-in" bonds to connect their end points; since we force these bonds to be in the tours, the renormalized problem is really a constrained TSP. The distance between two cities is the same as in the nonrenormalized problem if they are not connected by a frozen bond, otherwise their distance is given by the length of the subpath associated with the frozen bond. If this reduced problem is small enough, it can be solved by direct enumeration. Otherwise, we "open up the Russian doll" and solve this renormalized problem recursively. Since each parent is compatible with the selected patterns, each of them corresponds to a legal tour for the renormalized problem. Thus we can use these tours in the first generation of the recursive call of GRA: this way none of the information contained in the tours is lost.

How does one choose the number of parents k? Clearly, the tour parts that are shared by all k parents decrease as k grows and the child becomes less and less constrained. Increasing k then has the effect of improving the best possible child but also of making the corresponding search more difficult, so the choice of k results from a compromise. Genetic algorithms being biologically motivated, the choice k = 2 may seem natural, but it need not be optimal, and empirically we find it not to be. We do not claim to be the first to propose the use of more than two parents [11], but in previous proposals, the performance turned out to be lackluster. The reason is that they did not include the two essential ingredients: (i) a selection of patterns; (ii) a search for the best child consistent with the given patterns.

A bird's eye view of our algorithm is as follows. We start with a population of M randomly generated tours; a simplified version of the Lin-Kernighan (LK) [12] local search algorithm is applied to these tours which form the first generation. To obtain the next generation, we first produce by recursion as many children as there are parents; then the local search improvement is applied to these children; finally, duplications among the children and children which present no improvement over their worst parent are eliminated. The next generation consists of the children remaining. The algorithm terminates when there is only one individual left.

If the local search is taken as given (and we are not concerned here about its detailed implementation), our algorithm has two parameters, the number M of tours used in the population and k the number of parents of a child. In our numerical experiments for the TSP, we have chosen M = 50 for the topmost level where we treat the initial TSP instance, and M = 8 for the inner levels where renormalized instances are treated. Of course, other choices are possible, but we have not explored them much. Let us just note that it is desirable to have M large enough to have plenty of diversity in the patterns which will be selected, thereby increasing one's chance of finding the ground state. However, there is a high computational cost for doing this, as each level of the recursion increases the CPU time multiplicatively. Thus the best strategy would probably be to have *M* decrease with the level of the recursion. Concerning the choice of the parameter k, a similar compromise has to be reached. The best quality solutions would be obtained with large k, but this would lead to many levels of recursion and thus to very long computation times. In practice, we increase k dynamically until, of the current number of bonds to be found, at least a threshold fraction of 10% remains unfrozen at this step. This ensures that the renormalization does not reduce the problem size too dramatically, allowing good solutions to be found. For the instances we considered, nearly all values of k were between 2 and 6, with 5 being the most probable value.

How well does the method work? For the TSP, it is standard practice to test heuristics on problems from the TSPLIB library [13]. We have tested our algorithm on five problems of that library for which the exact optima are known. As can be seen in Table I, the improvement over the local search is impressive (we use a DEC- α -500 work-station to treat these instances). Still better results could be obtained by improving the local search part. Several other groups (see [4] and Chap. 7 of [8]) have fine tuned their LK algorithm both for speed and for quality. In spite of the fact that our version of LK is far less effective, we obtain results comparable to theirs. We believe that this excellent performance is possible because GRA incorporates the essential ingredients which allow the

TABLE I. Tests on 5 instances from TSPLIB; the number in the name of an instance represents its number of cities. Δ_{LK} and Δ_{GRA} are the relative differences between the length found by the corresponding algorithm and the optimum, τ_{LK} and τ_{GRA} are the CPU times in seconds to treat one instance, and P_{GRA} represents the probability for GRA to find the optimum. Data for the GRA have been averaged over 10 runs.

Instance	$\Delta_{ m LK}$	$ au_{ m LK}$	Δ_{GRA}	$ au_{ m GRA}/ au_{ m LK}$	$P_{\rm GRA}$
pcb442	1.9%	0.09	0%	2442	100%
rat783	2.0%	0.19	0%	2923	100%
fl1577	15.4%	0.63	0.0022%	3805	80%
pr2392	2.7%	0.98	0.0056%	5278	20%
rl5915	3.6%	3.94	0.013%	8202	0%

optimization to be effective on all scales. To give evidence of this, we now show that GRA is also extremely effective on a very different problem.

The spin glass problem (SGP).—Spin glasses have long been a subject of intense study in statistical physics. One of the simplest spin glass models is that of Edwards and Anderson [14] in which Ising spins ($S_i = \pm 1$) are placed on a lattice and the interactions are between nearest neighbors only. The corresponding Hamiltonian is

$$H = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j$$

where the J_{ij} are quenched random variables with zero mean. For our purpose here, the spin glass problem consists of finding the spin values which minimize H. To find this minimum with a genetic algorithm approach, we need the "building blocks" of good configurations. This time, simply looking at the variables (spin orientations) which are shared between parents is not effective since the energy is unchanged when all the spins are flipped. Instead, we consider correlations among the spins. The simplest correlation, whether two neighboring spins are parallel or antiparallel, will suit our needs just fine. Consider first any set of spins; if the relative orientations of these spins are the same for all k parents, we say that they form a "pattern"; the values of the spins in that pattern are then frozen up to an overall sign change. Now we sharpen a bit this notion of a pattern: we require the set of spins to be both maximal and connected, and we call such a set a block. (Note that the patterns introduced for the TSP also had these two properties.) We can associate a fictitious or "blocked" spin to each such block to describe its state. Flipping this blocked spin corresponds to flipping all the spins in the block, a transformation which maintains the pattern (i.e., the relative orientations of the spins in the block).

With these definitions, it is not difficult to see that each spin belongs to exactly one block (which may be of size 1 though). Furthermore, the configurations compatible with the patterns shared by the k parents are obtained by specifying orientations for each blocked spin; this procedure defines the space spanned by all possible children. Not surprisingly, the energy function (Hamiltonian) in this space is (up to an additive amount) quadratic in the blocked spin values, so finding the *best* possible child is again a spin glass problem, but with fewer spins. Because of this property, the renormalization and/or recursion approach can be used very effectively, similarly to what happened in the case of the TSP.

To find the (renormalized) coupling between two blocked spins, proceed as follows. First put the two spins in the up state; unblock each spin so that one has all the spins of the initial system they are composed of. The coupling between the two blocked spins is obtained by summing the $J_{ij}S_iS_j$ where S_i belongs to the set defining the first spin and S_j to that of the second. [Here, S_i denotes the value (±1) of the spin *i* when its (unique) blocked spin is up. Note also that to obtain the total energy of a blocked configuration, one also has to take into account the energy inside each blocked spin.] Finally, a straightforward calculation shows that this formalism carries over in the presence of an arbitrary magnetic field also.

Given the construction of blocks and a local search routine [we use a version of the Kernighan-Lin (KL) [15] algorithm], the GRA proceeds as before. For the number of parents k, we follow the spirit of the procedure used for the TSP: we increase k dynamically until the size of the renormalized problem is at least 7.5% that of the current problem. For this choice, k = 5 is the most frequent value, and we find that the distribution of k is rather narrow. (Clearly, when k increases, the size of the renormalized problem increases rather rapidly.)

Testing the algorithm is not easy as there is no library of solved SGP instances. Fortunately, when the grids are two dimensional, there are very effective exact methods for finding the optimum [16]. We thus performed a first type of test where we ran our GRA on ten instances corresponding to toroidal grids of size 50×50 with $J_{ii} = \pm 1$. (The exact solutions were provided by J. Mitchell.) For these runs we set M = 5 + 0.2N for each level (N being the number of spins at that level). The algorithm halted on the 6th, 7th, or 8th generation, and in all cases found the exact optimum. Furthermore, we measured the mean excess above the optimum for each generation. The first generation corresponds to simply using the local search, and had a mean excess above the optimum of 12%. Thereafter, the mean excess energy decreased by a factor of 2 to 3 at each generation, until it hit 0. (Furthermore, instance to instance fluctuations were small.) In terms of computation time, our local search took on average 0.02 sec on these instances, and the average time taken by GRA was 16,000 sec. This performance is competitive with that of the state of the art heuristic algorithm [17] developed specifically for the SGP. Since this same property was found to be satisfied in the case of the TSP, there is good evidence that GRA is a general purpose and effective optimization strategy.

As a second kind of check on our method, we considered three-dimensional grids of size $L \times L \times L$ with Gaussian J_{ii} 's for which exact methods are not so effective. These kinds of grids are of direct physical relevance [1]. Since we did not know the exact optima, our analysis relied on self-consistency: we considered we had found the optimum when the most powerful version of our algorithm (large M) output the same configuration with a probability above 90%. Measuring this probability requires performing many runs, but once one has this putative optimum, one can measure the performance of the algorithm in a quantitative way. To achieve the precision required we set M = N for the top level and M = 5 + 0.2N for inner levels, then the probabilities to find the optimum are as given in the last column of Table II. We also give in this table the performance of the GRA with M = 15 for all the

TABLE II. Tests on $L \times L \times L$ SGP instances. Δ_{KL} and Δ_{GRA} are the relative differences between the energy found by the corresponding algorithm and the optimum, τ_{KL} and τ_{GRA} are the CPU times in seconds to treat one instance. τ_{GRA} and Δ_{GRA} are results for M = 15. P_{GRA^*} represents the probability for GRA to find the optimum when M = N at the top level and M = 5 + 0.2N for inner levels.

L	Δ_{KL}	$ au_{ m KL}$	Δ_{GRA}	$ au_{ m GRA}/ au_{ m KL}$	P_{GRA^*}
4	8.2%	$7.9 10^{-4}$	0.087%	19	99.8%
6	11.5%	$1.5 \ 10^{-3}$	0.65%	43	98.6%
8	13.5%	$2.7 \ 10^{-3}$	1.09%	85	98.0%
10	14.1%	$7.1 \ 10^{-3}$	1.26%	104	94.0%

levels; for this choice of M, the algorithm is 1 to 2 orders of magnitude slower than KL, but leads to mean energy excesses that are 10 to 100 times smaller. Overall, the quality of the solutions is excellent even with a relatively small M, and we see that up to 1000 spins GRA is able to find the optimum with a high probability provided M is large enough.

For both the traveling salesman and the spin glass problems, our genetic renormalization algorithm finds solutions whose quality is far better than those found by local search. In a more general context, our approach may be considered as a systematic way to improve upon state of the art local searches. A key to this good performance is the treatment of multiple scales by renormalization and recursion. The use of a population of configurations then allows us to selfconsistently optimize the problem on all scales. Just as in divide and conquer strategies, combinatorial complexity is handled by considering a hierarchy of problems. But contrary to those strategies, information in our system flows both from small scales to large scales and back. Clearly such a flow is necessary as a choice or selection of a pattern at small scales may be validated only at much larger scales.

In this work, we put such principles together in a simple manner; nevertheless, the genetic renormalization algorithm we obtained compared very well with the state of the art heuristics specially developed for the problems investigated. Improvements in the population dynamics and in the local search can make our approach even more powerful. We thus expect genetic renormalization algorithms to become widely used in the near future, both in fundamental [18] and applied research.

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