Simulated Annealing for Spin-glass-like Optimization Problems

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The technique of simulated annealing has arisen from the comparatively large research effort devoted over the past 15 years to the understanding of spin glasses. The technique has already had a strong impact on combinatorial optimization and its applications. As an example, in this article I describe the relations between spin-glass theory and experiments on the one hand, and the computer-aided chip design of electronic circuits on the other. In that context, simulated annealing was first introduced by S. Kirkpatrick *et al.* [1]. To understand the approach, let us first take a closer look at the area of physics where it was first developed.

Spin-Glasses

As some readers may recall [see *Europhys. News* **14** (1983) 12], spin glasses are disordered alloys with magnetic ions coupled by the so-called RKKY pair interaction, which exhibits damped oscillations as a function of the separation between two spins. Classic examples are $Gd_{1-x}Mn_x$ and $Au_{1-x}Fe_x$. Such systems are described by the Hamiltonian

$$-\beta \mathcal{H} = \sum_{<i,j>} J_{ij} S_i S_j . \qquad (1)$$

We concentrate here on short-range Ising-spin models ($S_i = \pm 1$) with only nearest-neighbour couplings on either a square or a cubic lattice. Glass-like properties will arise if the interactions J_{ij} are assumed randomly distributed with zero mean either between $\pm J$ or according to a Gaussian. For recent reviews, see Refs. 2–4.

A fundamental characteristic of spin glasses is their "frustration" or high ground-state degeneracy, usually accompanied by a large number of metastable states close in energy. These properties are illustrated by the (free-) energy "landscape" shown in Fig. 1, where X denotes a representative coordinate in phase space, and E the corresponding energy. Relatively high barriers separate different valleys. The bottoms of the valleys correspond to the above-mentioned ground states or metastable states. The key conjecture is that this picture also applies, at least qualitatively, to a wide variety of complex optimization problems in everyday life.

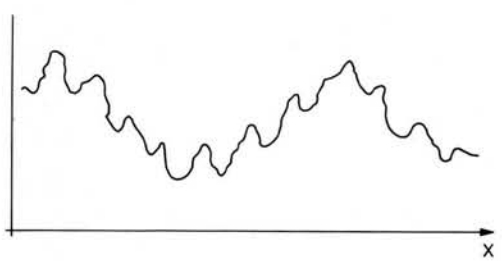

Fig. 1 — Schematic phase space cut through free energy landscape.

NP-Complete Optimization Problems

"NP-complete" describes a class of problems such that the computing time necessary to construct an optimal solution increases faster than any power of N (the number of basic elements or spins); therefore they are called Non-(deterministic) Polynomial. "Completeness" refers to problems of a given class that can be mapped onto each other in polynomial time. The search for a ground state in a spin glass belongs to the former class in the case of a three-dimensional lattice. The two-dimensional case only is P-complete. Other famous NP-complete problems are the "Travelling Salesman" and the "Placement and Wiring" of gates in chip design. As we shall see later, a huge variety of such problems exists in economics, biology, engineering, *etc.* In general, we can establish a connection between the "cost function" of an optimization problem and the total interaction energy of a spin-glass. In one obvious case, the cost function is the amount of money a travelling salesman has to spend to visit N cities, one after the other. In placement and wiring problems, it is the wire length L and/or the size of the chip.

Heuristic methods have already been developed for many such practical optimization problems. However, each such method is specially designed for a given problem and is therefore rather restricted in scope. In contrast, the "simulated-annealing" method provides a quite general approach. Annealing means controlled thermal treatment followed by slow cooling. For spin glasses, judicious "cooling" procedures have been developed to obtain ground-state configurations in computer simulations [2].

Chip-Design for Physicists

The placement or interconnexion problem for chips illustrates in a nutshell the simulated-annealing technique. Two-dimensional gate arrays are commercially available and consist of a certain fixed number of "cells" (for instance 2000) built from several transistors that perform a particular logical function. These cells are implemented on the gate array, and have to be wired by the user according to the logic of the chip which is specified in a "netlist". In view of the finite speed of electromagnetic signals, the chip performance depends critically on the total wire length L. Excessive congestion resulting in local overheating is a related problem to be avoided. Therefore, the total wire length is the cost function to be minimized. In view of the apparently large number of possibilities, this is done by the following Exchange Algorithm (see Fig. 2): Two cells are selected at random, and their positions exchanged. The difference in wire length ΔL is calculated. To avoid getting stuck prematurely in a metastable minimum, the disadvantageous configuration is not rejected automatically. Instead, it is assigned a probability P and the exchange will be accepted if P exceeds a number chosen randomly between 0 and 1. The acceptance probability for the basic move is calculated according to the Monte-Carlo rule used to compute thermal equilibrium properties of interacting systems in classical statistical mechanics,

$$P = \exp(-\Delta L/T) \quad \text{for } \Delta L \geq 0$$
$$P = 1 \quad \text{otherwise,} \qquad (2)$$

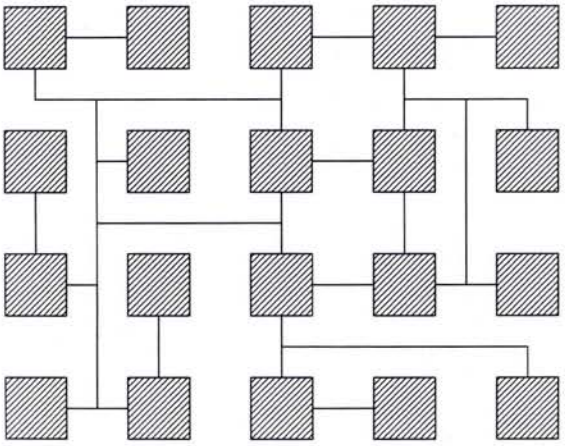

*Fig. 2 — Schematic two-dimensional gate array. Logic cells (squares) are connected by wires. From Morgenstern I. and Würtz D., Z. Phys. B **6/7** (1987) 397.*

where T is a fictitious temperature. After a large enough number of exchanges, the system "equilibrates" by spending most of the time in configurations with low values of L. To find one with minimum L, the system is "annealed" by slowly lowering T in small increments. In spin-glass models, the analogous basic move is simply the flipping of a spin at a particular lattice site. The analogy to spin glasses can be fruitfully pursued. Thus, the emergence of a preferred wiring configuration is monitored by considering the mean square fluctuation of the wire length

$$C = <L^2> - <L>^2 \qquad (3)$$

as a function of T. It is natural to compare this quantity with its analogy in statistical mechanics which is proportioned to the specific heat. For the three-dimensional $\pm J$ spin glass, extensively investigated on a special-purpose computer at AT&T Bell Laboratories, we notice a broad rounded peak on a *linear* temperature scale (Fig. 3a). A similar picture is obtained for the chip-design problem, but on a *logarithmic* scale, as seen in Fig. 3b. The corresponding annealing was performed according to the logarithmic cooling rule

$$T_{new} = \alpha \cdot T_{old}, \qquad (4)$$

where $\alpha = 0.8-0.9$.

In the chip-design case, this may also produce a second peak denoted by "clustering" [1]. The simulation first singles out clusters of strongly connected cells that are absent in short-range spin-glass models. At lower temperature, "ordering" takes place, optimizing interconnexions inside the clusters. In Fig. 3a, the critical temperature T_c for the three-dimensional spin glass is indicated. A finite critical temperature "T_c" is also found in the finite gate-array problem, although T_c vanishes for the short-range spin glass in two dimensions. Below this temperature, the system is "frozen", *i.e.* the correlation length becomes comparable to the system size.

Annealing Schedule

The behaviour of the specific heat suggests a more efficient annealing schedule. This proposal is influenced by experience gained in spin-glass simulations. Here, we started at a high enough temperature (see Fig. 3a) where the specific heat is relatively low because no large energy fluctuations occur as the system has a mean energy well above the peaks in Fig. 1. The above-mentioned critical temperature plays an important role. As T is decreased below T_c, the annealing procedure selects a particular, wide valley in phase space (Fig. 1) out of which the system can subsequently no longer escape. The closer we are to equilibrium just above T_c, the more reliable our final result. In spin-glass-like problems, "T_c" is usually located on the low-T side of the specific-heat peak. A good rule of thumb is to decrease the cooling rate between the peak of the specific heat and the position of T_c by a factor of at least 10 to 20. Below T_c, the cooling rate can be increased to its initial value: The remaining small subsidiary valleys still have a chance to be explored before the system is completely "frozen" in an absolute minimum configuration. Whether one should cool linearly or logarithmically, or according to some other rule, is answered by exploiting the resemblance of the "specific heat" for chip desing and spin glasses. The temperature dependence of this quantity can be computed relatively quickly, as it is dominated by frequent small-amplitude fluctuations. A rounded peak is a clear indication for "spin-glass-like" behaviour. Summarizing extensive experience, I recommend the following procedure:

(i) Plot the specific heat against a modified temperature scale which gives a spin-glass-like peak with comparable width.

(ii) Start annealing well above the peak. Take equidistant points on the new temperature scale.

(iii) Cool slowly between the peaks down to "T_c" as outlined above. A conjecture by Grest *et al.* [5] deserves mention at this point. They looked at the cost-function value reached at the end of an annealing schedule as a function of the cooling rate. Studying mainly spin-glass models, they obtained

$$E(\tau) \sim 1/\ell n \tau \qquad (5)$$

where τ is the time spent in each temperature interval and E is referred to its ground-state (optimum) value. This result is still hotly debated, especially in the spin-glass community [4]. Nonetheless, it or a modified scaling law would provide an answer to the most important question in simulated annealing. How much computing time must be spent to obtain a useful solution to an NP complete problem?

Engineering Applications

Simulated annealing has been used in a variety of problems. The strength of the method is certainly its generality. In principle, simulated annealing can be applied to all problems which can be attacked by iterative improvement [1]. Several such problems are described by Dreyfus *et al.* in Ref. 4, which presents a current overview of the situation. They include cloth cutting, time scheduling, planning of office buildings, and warehouse management.

More difficult tasks considered by the same authors include so-called "inverse

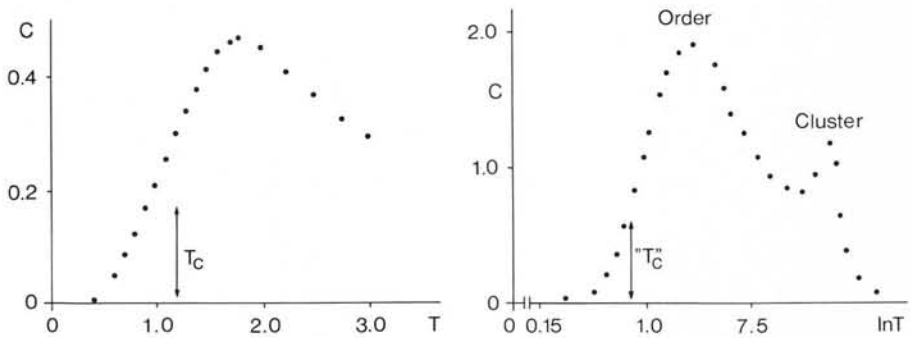

Fig. 3 — Computed specific heat of (a) three-dimensional spin-glass model (linear temperature scale), and (b) chip-design problem (logarithmic temperature scale). From Morgenstern I. and Würtz D., Z. Phys. B, to be published. © Springer-Verlag 1987.

problems". An example is image processing where one tries to reconstruct the original and not just any acceptable optimal solution or image. One of the most spectacular applications is the interpretation of seismic data by Rothman [6]. He was able to reconstruct the geological structure of a terrain from information on the propagation of sound waves. Other impressive applications involve the reconstruction of three-dimensional objects from two-dimensional images in tomography, and the deblurring of binary images.

Conclusion

Simulated annealing offers a rather general approach to time-consuming problems. This is on the one hand its strength but on the other hand also its weakness. That means problem-oriented heuristic approaches may exist which are hard to beat. The general rule seems to be: the more money at stake in the solution of a particular problem, the better is the existing heuristics. This is certainly the case in chip design, where a general breakthrough for simulated annealing has not happened so far. But further research aims at this goal [4]. For a huge variety of less popular problems, simulated annealing is the way to proceed. In such a case, I encourage the reader to try my recipe. If the problem turns out to be "spin-glass-like", a comparatively good solution can be obtained for an optimal state. The future of simulated annealing certainly lies in the large variety of such problems waiting to be discovered in all branches of science, technology and economics.

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