0.0 ABSTRACT.
Finding a global optimum value for an objective function with many degrees of freedom subject to conflicting constraints is a combinatorially explosive problem. This paper will review an approach to these types of problems based on an analogy to concepts in statistical mechanics. A SAS version of the algorithm is used to solve the Traveling Salesman Problem. These techniques have proved to be useful in VLSI design and are the basis for several Neural Network algorithms currently being used to solve AI problems. Applications and limitations of these techniques are reviewed.

1.0 INTRODUCTION.
A typical optimization problem requires that some objective function be minimized or maximized over some N dimensional space. If the N input parameters are continuous variables the solution technique usually involves some form of hillclimbing. The combination of input parameters are varied so that the solution search continues uphill or downhill in a favorable direction. These techniques are sometimes referred to as gradient descent.

If the input parameters are discrete the input configuration space may not have any identifiable direction. In this case some method must be used to discover a combination of input parameters that will result in a good solution.

It is usually not possible to exhaustively explore the solution space. The combinations of input parameters increases exponentially with the size of the problem. This is characteristic of a class of similar problems. For problems of significant size, optimal solutions in a reasonable time are not obtainable with even the fastest computers. Relatively good solutions can often be found by using heuristic algorithms.

Recently several new approaches have been developed based on analogies to physical phenomena. These "natural techniques" include Simulated Annealing (13), Genetic Algorithms (9), and Neural Networks (11,2,8). This paper focuses primarily on simulated annealing.

2.0 THE ENERGY ANALOGY
The simulated annealing technique solves combinatorial optimization problems by using an analogy from physics. Statistical mechanics predicts the behavior of large systems of interacting components.
3.1 TSP-TYPE PROBLEMS

One of the most widely analyzed examples of combinatorial optimization is the Traveling Salesman Problem (TSP). In this problem, a traveling salesman must visit, only once, each of N cities. The objective is to find the shortest route possible. This problem is discrete, combinatorially explosive and subject to local minima. TSP is related to similar problems such as vehicle routing and some forms of scheduling problems. This problem can be formulated by using the energy analogy:

1. A starting configuration is chosen randomly or by some fast heuristic algorithm. A tour is represented as some permutation of the N cities to be visited. This constitutes an initial tour which is to be improved by some version of a tour improvement algorithm.

2. Thermal equilibrium is represented by finding a suitable number of rearrangements at each temperature level. Two types of rearrangements have been suggested (17). A section of the tour can be reversed. An alternative is to move a section of the tour to another location.

3. The energy function is taken to be the distance function. (for some applications the metric might be cost, delay etc.)

\[ E = \text{Distance} = \sum_{i=1}^{N} \sqrt{(X_i - X_{i+1})^2 + (Y_i - Y_{i+1})^2} \]

4. An annealing schedule requires some arbitrary control parameter T analogous to temperature. T must be set to a relatively high value and be reduced by a step size S. A typical temperature reduction is to multiply the temperature by .9 at each step. At each level of T, rearrangements should be tried. The number of rearrangements can be limited by the number of successful rearrangements or by the amount of reduction in the energy level. There is no general agreement on the best choice of T, S and R. Kirkpatrick (13) used this general approach and has suggested using quantities analogous to entropy and specific heat to guide the TSP solution search. The adjustability of the annealing parameters allows the possibility of controlling solution quality that ranges from that of the starter heuristic to the absolute optimum.

3.2 VLSI

The most well known use of Simulated Annealing is the application to VLSI design by IBM physicists. (23) In this case the objective was the minimization of connection lengths between electrical elements while balancing the allocation of connections to minimize interference and to allow maximum flexibility for additions and revisions. Simulated Annealing, with problem specific heuristics, improved random routing by approximately 57 percent.

3.3 COMMUNICATIONS NETWORKS.

Many network problems such as topological design and routing are known to be combinatorially explosive. Many network heuristic network algorithms are markedly suboptimal. Regardless of whether they are fast or slow these algorithms typically provide solutions at only one level of quality. There are a great many opportunities in this area to use stochastic relaxation to improve problem solutions.

4.0 RELATIONSHIP TO NEURAL NETWORK ALGORITHMS.

There has recently been a resurgence of activity in the area of neural networks A series of articles in AI expert magazine provides an primer on Neural network techniques (2). The variety of neural network algorithms share a common theme; the establishment of weights on connections between nodes. It was recognized by Hopfield (10) that Neural Network models could be viewed as a search for minima on an energy surface. Hopfield and Tank used Neural Networks to solve the TSP (II). The initial approach was susceptible to local minima traps. This lead to the development of the Boltzmann Machines. (8)

4.1 BOLTZMANN MACHINES

Boltzmann Machines introduce a form of simulated annealing into Neural Network algorithms. A variation of the Metropolis Algorithm is used to determine the output of a Neural Network element:

\[ \frac{1}{1 + e^{-\frac{\Delta E}{kT}}} \]

The shape of the energy function is determined by the weights of the connections between nodes. Neural networks have the capability to learn the shape of the energy function. Stochastic relaxation provides the capability to tolerate imprecise (noisy) input.

4.2 HARMONY THEORY

Another Neural Network technique, Harmony theory also incorporates a similar relaxation technique. For a comparison of Boltzmann machines and Harmony functions see Smolensky (22).

5.0 SAS IMPLEMENTATION

A project was initiated to study the effectiveness of Simulated Annealing in a SAS environment. The goal is to compare the performance of relaxation techniques with conventional algorithms for the same problem. The TSP is chosen as a suitable test problem. An interesting application of SAS to the TSP has appeared in SUGI proceedings (3). However Lins Heuristic (15) was chosen as the traditional heuristic benchmark for the following reasons:

1. The benchmark needs to be as fast and as efficient as possible.
2. The benchmark needs to be able to accept large problems (at least 20 to 100 nodes).
3. It is desirable to package the algorithms within a SAS PROC. (5, 12, 19)
Many researchers have reported finding solutions within 2-3 percent of the optimal lower bound for a large number of cities within seconds to minutes. Lins heuristic has an estimated 85 percent frequency of finding an optimum solution for 50 points randomly generated on the unit square. This frequency drops to 21 percent for 110 points. For large problems a level of confidence can be estimated for finding optimal solutions by repeated trials of Lins heuristic with random starting points. A more powerful algorithm for finding optimal tours has recently been discovered by Rinaldi and Padberg (18). The underlying principle is to use multiple random applications of a fast heuristic (Lins) to zero in on a subset of the solution space where the optimal tours are to be found. This algorithm combines Lins algorithm with 3 other techniques including some proprietary code. It does not appear practical to implement this algorithm as a SAS proc at this time.

The evaluation procedure is as follows:

1. Problem creation.
   - Select N random cities from Map dataset in SAS/GRAPH.
   - Use projected coordinates for node locations

2. Problem solution.
   - Exec (proc) TSPLIN to solve problem.
   - Exec (proc) TSPANN to solve problem.

3. Results analysis.
   - Use SAS/GRAPH to map tours as in (3).
   - Use SAS to analyze tour length vs control parameters for tuning TSPANN.
   - Use SAS/graph to display relative performance (21).

6.0 SUMMARY

6.1 LIMITATIONS

Stochastic relaxation techniques appear to be inherently slow. Some analysis has been done to determine the annealing schedule sufficient for convergence to optimal solutions. It has been shown(4) that to guarantee an optimal solution an inverse logarithmic temperature reduction is necessary:

\[ \text{Temp}(\text{step}+1) = \text{Temp}(\text{initial})^{(1/(1+\text{step}))} \]

This is probably too slow for many practical applications. Practical convergence may be faster than this theoretical upper bound(7).

The TSP has a particular characteristic not common to all combinatorial optimization problems. Any suboptimum solution contains the seeds of the optimum solution. Any proposed solution contains all the nodes in the original problem and is a permutation of the optimum solution. This may limit the generality of the results of analysis of the TSP.

6.2 EXTENSIONS

A strategy similar to Rinaldi-Padberg can be used. Use Lins algorithm, or some fast heuristic, to get close to the optimal tour. Then anneal this answer to the quality that you are willing to pay for (up to optimality).

Several ideas can be borrowed from recent developments in the Neural network area. One new technique is to preprocess the input data so that the minimization technique can be parameterized to fit the data. This could result in more appropriate annealing schedules. It has been been discovered that the Cauchy/Lorentzian distribution provides faster escape from local minima while preserving convergence (24). The generating function is:

\[ g(x) = \text{Temp}(\text{step})/((\text{Temp}(\text{step}))^{0.5} + x^{0.5}) \]

The temperature step reduction required for optimality is then:

\[ \text{Temp}(\text{step}+1) = \text{Temp}(\text{initial})^{(1/(1+\text{step}))} \]

This will permit faster annealing and increase the practicality of stochastic relaxation techniques. This technique has been compared in significance to the discovery of the Fast Fourier Transform (FFT).

6.3 RELATIVE PERFORMANCE

When "natural algorithms" are applied to Operations Research or Engineering problems traditional performance measures are more important than the "naturalness" of the algorithm. It is not yet clear that any stochastic relaxation technique can compete with the performance of Rinaldi-Padberg (or Lin) for solving the TSP. Also Barahona et al (1) suggest that the VLSI circuit design problem may have a fast solution using a traditional OR technique.

Initial testing has been somewhat disappointing. Development of a good annealing schedule appears critical. It is certainly easy to make annealing perform badly. This project is still ongoing and it is too early to draw final conclusions.

However, there several good reasons not to dismiss the relaxation techniques yet:

(a) There are still many areas for improvement.
(b) Many existing heuristics could benefit from relaxation. In general the faster the heuristic the less optimal is its solution.
(c) These techniques provide a tunable tradeoff between computational work and quality of solution.
(d) Stochastic relaxation techniques are increasingly important in Neural Networks algorithms which will rapidly speed up on parallel hardware.

6.4 DIRECTION

The current goals for this project are:

(a) Complete test with fast(Cauchy) simulated annealing.
(b) Complete analysis of practical vs optimal annealing schedules
(c) Completely embed all algorithms in SAS PROCs.
(d) Make code available.
(e) Possible refinements based on feedback from step d.
(f) Begin application to analysis of telecommunication networks.

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REFERENCES


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