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Theory and Methodology

An improved annealing scheme for the QAP

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Abstract: Recently there has been some interest in the use of Simulated Annealing to obtain 'good' solutions to a number of combinatorial problems. This paper reports on the use of this method applied to the Quadratic Assignment Problem (i.e. the assignment of inter-communicating objects to locations to minimize the total cost of communication between them). The result is a much-improved annealing scheme for this problem which performs well on a range of examples, finding improved solutions for several of the largest problems available in the literature and requiring only modest amounts of computational effort.

Keywords: Simulated annealing, heuristics

Introduction

Recently there has been some interest in the use of Simulated Annealing to obtain 'good' solutions to a number of combinatorial problems. The central idea of this method is that certain uphill steps may be required to prevent an optimization scheme from getting stuck in a poor local optimum.

For a particular problem one must specify a topology (or neighbourhood structure), and an efficient method of moving from one solution to a neighbouring one and computing the resulting change in the objective function. In general, improvements are always accepted while uphill moves are accepted with a probability which depends on the size of the increase and the state of a number of controlling parameters. Originally the method was used by Metropolis et al. [10] to simulate energy levels in cooling solids and Boltzmann's Law was used to determine the probability of accepting a perturbation resulting in a change δ in the energy at the current absolute temperature T, i.e.,

$$P(\text{accept}) = e^{-\delta/kT},$$

where k is Boltzmann's constant.

The temperature was initially set to some large value, thereby permitting almost all attempted moves and gradually lowered in a pre-determined fashion until no further change seemed likely and the system was considered to be 'frozen'.

These ideas have been applied to various combinatorial problems by a number of authors with slight variations in the cooling scheme and the setting of the various controlling parameters. Details will be given here of extensive trials of this method applied to a particular combinatorial problem, namely the Quadratic Assignment Problem (QAP) (i.e. the assignment of inter-communicating objects to locations to minimise the total cost of communication between them). The result is a much-improved annealing scheme for this problem which, even when using default values for all its parameters, performs well on a range of examples, finding improved solutions for several of the largest problems available in the literature.

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The Quadratic Assignment Problem (QAP)

In its most general form the QAP of size n can be formulated as

Minimise

$$\sum_{i=1}^{n}\sum_{a=1}^{n} B_{ia}\cdot x_{ia} + \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{a=1}^{n}\sum_{b=1}^{n} C_{ijab}\cdot x_{ia}\cdot x_{jb}$$

subject to

$$\sum_{i=1}^{n} x_{ia} = 1, \quad a = 1, 2, \ldots, n,$$

$$\sum_{a=1}^{n} x_{ia} = 1, \quad i = 1, 2, \ldots, n,$$

$$x_{ia} = 0 \text{ or } 1, \quad i = 1, 2, \ldots, n, \quad a = 1, 2, \ldots, n,$$

where B_{ia} is the direct cost of assigning facility i to location a and C_{ijab} is the cost incurred by the joint assignment of i to a and j to b. Often this cost is defined as the flow F_{ij} of some commodity from facility i to facility j times the distance D_{ab} from a to b. This is the case in all problems presented here.

As a notational convenience, note that any feasible solution can be represented by a permutation Φ of the integers from 1 to n where $\Phi(i)$ denotes the chosen location of facility i.

Applications of the QAP include Dickey and Hopkins' campus-planning [4], Elshafei's hospital lay-out [5], Steinberg's backboard wiring [14], and many others. (See [1] for a more extensive list of applications.)

Since current exact solution methods are only computationally feasible for very small problems ($n < 20$), much of the recent research work has been aimed at producing heuristics which can find 'good' solutions to larger problems in reasonable amounts of computer time. One such approach which has recently yielded promising results is the use of Simulated Annealing [3,16].

The following sections describe the author's investigation of this technique and his attempts to produce an improved annealing scheme which can perform well on a wide range of QAP's.

Investigation of the Annealing Method

All the versions of Simulated Annealing which have been used here start from a random permutation of the facilities. A neighbourhood move consists of swopping two facilities i and j and computing the resultant change in the objective function using the formula

$$\delta = B_{i\Phi(j)} + B_{j\Phi(i)} - B_{i\Phi(i)} - B_{j\Phi(j)} + 2\sum_{k\neq i,j}\left(\left(F_{jk} - F_{ik}\right)\left(D_{\Phi(i)\Phi(k)} - D_{\Phi(j)\Phi(k)}\right)\right).$$

Note that the use of this formula assumes that F and D are symmetrical.

All moves improving the current objective (i.e. $\delta \leqslant 0$) are accepted while uphill steps of size $\delta > 0$ are accepted with probability $e^{-\delta/T}$ by drawing a random number X from a uniform [0, 1] distribution and accepting the swop if $X \leqslant e^{-\delta/T}$. In all cases the *best* solution found during the search was recorded (as opposed to the one at which the scheme terminated).

The main differences in the methods tested are:

(i) How the attempted pair-swops are selected.

(ii) How the temperature is determined and controlled.

Random vs. sequential neighbourhood search

Most authors who have reported on the use of Simulated Annealing define a neighbourhood structure for their particular problem and choose the next potential solution *at random* from the set of neighbours of the current solution. However, it was felt that this approach might be inefficient for two reasons. Firstly, potential improvements might be missed at low temperatures because of the random nature of the search and secondly, attempts to move away from local optima could be thwarted by the premature repeal of uphill escape attempts. To explore this possibility, two annealing schemes were written which differed only in how the potential moves were selected. In the first, L&M1, two facilities are chosen at random, δ (the cost of swopping them) is computed, and the move is accepted or rejected by the standard negative exponential rule described above. In the second, L&M2, the potential pair-swops are examined in the order

$$(1, 2), (1, 3), \ldots, (1, n), (2, 3), \ldots, (n-1, n), (1, 2), \ldots$$

and so on, δ is computed and the swop is accepted

or rejected as before. In both cases the temperature is controlled by the Lundy and Mees [9] scheme were the temperature drops after each attempted pair-swop, from a specified starting temperature T_0 to a specified final temperature T_f by the recurrence relation

$$T_{i+1} = T_i/(1 + \beta T_i), \quad \text{where } \beta \ll T_0.$$

To enable comparison with order methods it is desirable that this cooling scheme could be completed in a specified number of steps M. This is achieved by setting $\beta = (T_0 - T_f)/MT_0T_f$.

Tests were carried out on the four largest Nugent et al. problems ($n = 12$, 15, 20 and 30) [11] and on eight new problems with random flow matrices (elements uniform on $[0,\ldots,100]$) combined with:

(a) the Nugent et al. rectangular-grid distances,

(b) new random distance matrices with elements uniform on $[1,\ldots,100]$.

Ten trials were performed on each of these problems with M, the number of swops examined, equal to $50K$ (where $K = \frac{1}{2}n(n-1)$ is the size of the neighbourhoods), and T_0 and T_f equal to the largest and smallest (non-zero) uphill steps found in 10 000 previously performed swops. (Many other parameter settings were tried and found to give similar results. Precise details are omitted for the sake of brevity.) The best solutions found and average deviation from the best known cost are recorded in Table 1. (The best known costs for the new problems used here were found during more extensive trials of the Q8-7 scheme described below.)

Applying the Wilcoxon signed rank test (e.g. [7, p. 211]) to the average deviations shows that the superiority of L&M2 over L&M1 is significant at a 98% confidence level. Therefore it is clear that for this class of problem a sequential neighbourhood search results in an improved annealing scheme.

Note that it is only the fact that the neighbourhoods are explored thoroughly that is significant —the actual order in which the possible pair-swops are generated is not important. Similar results were obtained when the list of pair-swops was initially 'shuffled' once before being used. In fact this approach may be superior for other problems in which the 'natural' ordering causes the search to perform badly. Random search-without-replacement techniques could probably achieve the same effect, but at the expense of slightly more computational effort.

Temperature control

Now attention was turned to the temperature controlling mechanism. In an attempt to discover whether or not cooling slowly from a high temperature to a low one is necessary, a scheme was

Table 1
Comparison of ordered and random search strategies averaged over 10 starts

Problem	Best known solution	L&M1 (Random)		L&M2 (Ordered)	
		Best found	Ave% dev	Best found	Ave% dev
Nf12×Nd12	578	578	2.42	578	1.56
Rf12×Nd12	12500	12500	1.43	12500	1.19
Rf12×Rd12	263058	263058	2.26	265146	2.41
Nf15×Nd15	1150	1160	2.03	1150	1.10
Rf15×Nd15	22972	23096	1.01	22972	0.71
Rf15×Rd15	409826	417156	4.41	422410	4.07
Nf20×Nd20	2570	2580	2.16	2574	1.59
Rf20×Nd20	50058	50160	1.49	50414	1.21
Rf20×Rd20	729884	748426	4.21	743748	4.09
Nf30×Nd30	6124	6154	1.52	6138	1.05
Rf30×Nd30	139640	140084	1.11	139968	0.85
Rf30×Rd30	1757188	1813230	4.42	1810000	4.41
			Average = 2.37		Average = 2.02

written which performs the entire search at a constant temperature specified by the user. No convergence is required—the algorithm examines M potential swops (chosen in order as in L&M2) and stops. This scheme was called FXDT2.

Averages of the scores obtained in 100 trials on the three Nugent et al. problems were computed for a range of fixed temperatures and the results are illustrated in Figure 1. Clearly if the system is kept too 'hot' then too many bad uphill moves are accepted for any good solution to be reached while if it is too 'cold' then the scheme will quickly drop into a local optimum and the remainder of the search will be a fruitless attempt to escape from it. Thus we would expect that somewhere between these two extremes there must be an optimum fixed temperature. What is surprising is how effective the search becomes at this optimum temperature (see Table 2). Further tests revealed that the value of the optimum temperature was little affected by the number of swops used to determine it and that, by and large, the more of a standard annealing search performed at, or close to, the optimal temperature, the more successful that search became.

The possible existence of a optimal temperature raises another problem—How can it be located? It may be that the user will need to solve sufficiently many similar problems on a regular basis to justify the overhead of initially performing numerous trials over a range of temperatures to determine the optimum value. However, it was felt that a more refined approach was necessary.

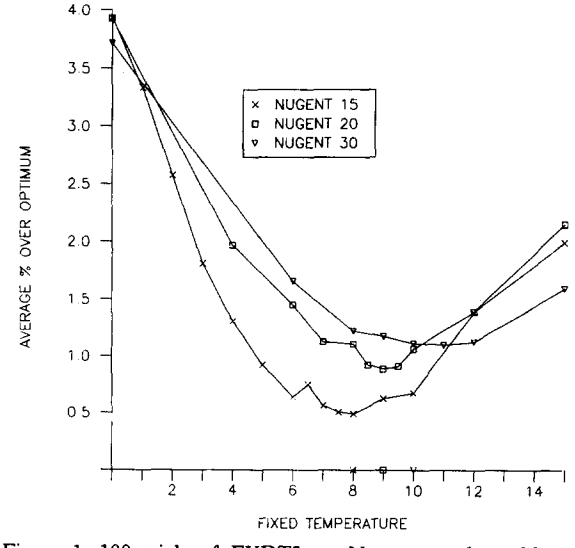

Figure 1. 100 trials of FXDT2 on Nugent et al. problems ($M = 50K$)

Table 2
100 trials of FXDT2 on the three largest Nugent et al. problems

N	15	20	30
M	5250	9500	21750
T^*	8	9	10
Best known solution	1150	2570	6124
Best solution found	1150 [a]	2570 [b]	6128
Average % deviation	0.49	0.88	1.11
Proportion within 1% of optimality	0.88	0.58	0.47
CPU secs per start on a VAX 11/785	2.38	5.43	19.70

[a] Achieved 22 times.
[b] Achieved 13 times.

Kirkpatrick et al. [6], and Vanderbilt and Louie [15] suggest that a peak in the 'specific heat' $C(T)$,

$$C(T) = \frac{\mathrm{d}}{\mathrm{d}T}\langle E(T)\rangle = \frac{\langle E(T)^2\rangle - \langle E(T)\rangle^2}{T^2},$$

(where $\langle E(T)\rangle$ is the average value of the objective at temperature T) is an indicator of a critical temperature where 'very slow cooling is required'. However limited tests exploring this idea failed to reliably predict the optimal temperatures as determined empirically above. Therefore a more prosaic approach was adopted. A new annealing scheme (Q8-7) was written to try to maximise the proportion of the search performed near an (unknown) optimal temperature. (The name of this scheme derives from the fact that it was the seventh modification of the eighth annealing scheme tested on the QAP by the author!) The scheme is as follows.

By a suitable choice of M, the number of swops examined (in order, as in L&M2), the user can easily control the running time of the algorithm. The default value of M is $M = 50K$ (where $K = \frac{1}{2}n(n-1)$, the number of neighbours of each point).

If the user does not specify a temperature range, then $\frac{1}{100}M$ random swops are used to determine $\delta_{\max}$, $\delta_{\min}$ and T_0, T_f are given the values

$$T_0 = \delta_{\min} + \tfrac{1}{10}(\delta_{\max} - \delta_{\min}),$$
$$T_f = \delta_{\min},$$

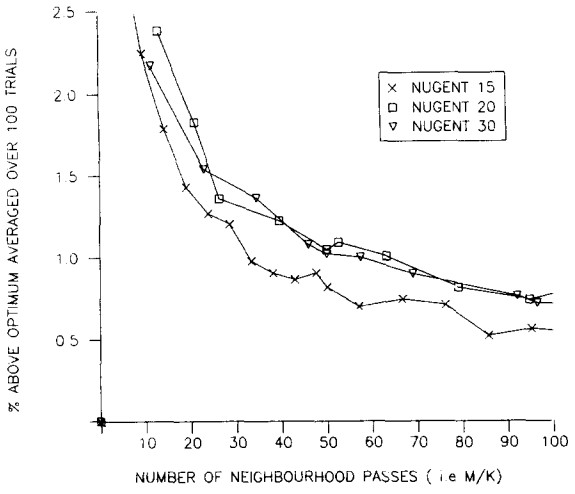

Figure 2. Q8-7 on Nugent et al. ($n = 15$, 20 and 30) problems

i.e. only the bottom tenth of the range of temperatures used in the schemes above. Thereafter the temperature is controlled as in L&M1 except that if MXFAIL consecutive uphill steps are rejected, then

(i) the next uphill is accepted,

(ii) T is returned to TFOUND, the value at which the current best solution was found, and

(iii) cooling is stopped by setting $\beta = 0$.

The aim of this scheme is that TFOUND will be a reliable indicator of the optimal temperature. MXFAIL is an adjustable parameter but in all results quoted here it has its default value of $\frac{1}{2}n(n-1)$ (which is K, the number of neighbours of each point).

Results for the three largest Nugent et al. problems are illustrated in Figure 2. (N.B.: The time per pass for the $n = 15$, 20, 30 problem is approximately 0.049, 0.110, 0.375 CPU seconds respectively on a VAX 11/785.)

Further improvement can be achieved by adding a post-analysis routine which performs an efficient down-hill search on the best solution found during the annealing search. (N.B.: The resulting algorithm, Q8-7B, no longer satisfies the condition that the CPU time required is proportional to M since a short annealing search requires more effort in the downhill phase to reach a local optimum.)

Q8-7B was run 100 times with default parameters on the three largest Nugent et al. problems, the Steinberg ($n = 36$) back-board wiring problems with both Euclidean and Rectilinear distances [14], and the two new problems generated by Wilhelm and Ward [16] ($n = 50$ and $n = 100$). The results are given in Table 3. Note that Q8-7B frequently betters the best published solutions for the $n = 50$ and $n = 100$ problems [16] and almost always finds a solution within 1% of the new best known solutions (although how close these are to the true optima is still open to question). Note also that, in common with other exchange procedures, Q8-7B performs less well on the Steinberg problem than on other problems of comparable size because of the high 'flow-dominance' of this problem (see [8,13] for further discussion of this phenomenon), but it still managed to find an improved solution to the rectilinear distance version.

Table 3
100 trials of Q8-7B on a range of problems in the literature. (Number of swops examined = $50K$)

Problem	N	Best known objective	Best objective found	Average % deviation	No. within 1% of opt	CPU per start on VAX 11/785
NUG15	15	1150	1150	0.74	67	2.46
NUG20	20	2570	2570	0.82	49	5.68
NUG30	30	6124	6124	0.95	59	18.68
STB(ED)	36	4119.55 [a]	4130.14	3.96	4	33.21
STB(RD)	36	4768 [b]	4768	4.39	3	33.00
W&W50	50	48816 [c]	48842 [d]	0.39	95	93.66
W&W100	100	273400 [c]	273454 [e]	0.31	100	734.58

[a] Reported in [12].
[b] Previous best published score = 4774 [2].
[c] Found during subsequent trials of Q8-7B.
[d] 62 out of the 100 trials achieved scores better than the previous best published score (i.e. 48944 in [16]).
[e] 28 out of the 100 trials achieved scores better than the previous best published score (i.e. 274022 in [16]).

Comparison of annealing schemes

How well does Q8-7 compare with other annealing schemes? In 1984, Burkard and Rendl [3] suggested an annealing scheme for the QAP in which the temperature is held fixed for a number of potential (randomly chosen) swops before being dropped so that cooling takes place in a series of jumps. The process continues until no (non-zero) change in the objective function is accepted at a particular temperature. The parameters required by this scheme are T_0, the initial temperature, L, the number of swops examined at each temperature and α, the multiplicative factor used to reduce the temperature.

A variety of L's and α's were tried but no clearly dominant strategy emerged. Results quoted here are for $L = \frac{1}{2}n^2$ with the choice of α used to control the total number of swops examined. Burkard and Rendl give no precise rule for determining T_0 other than to 'set T to an appropriately high value'. It was decided to set $T_0 \approx \delta_{max}$, the largest uphill step found in 10000 random swops performed previously, thereby giving an initial probability slightly greater than $\frac{1}{3}$ ($e^{-1} \approx 0.368$) of accepting such a move. This scheme is called B&R1. In [3] the authors also suggest a slight modification to this scheme in which the loopsize L (i.e. the number of swops attempted at each temperature) is multiplied by 1.1 after each loop so that more swops are attempted at the lower temperatures. This scheme is called B&R2. Again only results with the initial loopsize ($\frac{1}{2}n^2$) are given here, as a representative sample of the trials performed. Other details are as in the B&R1 scheme above.

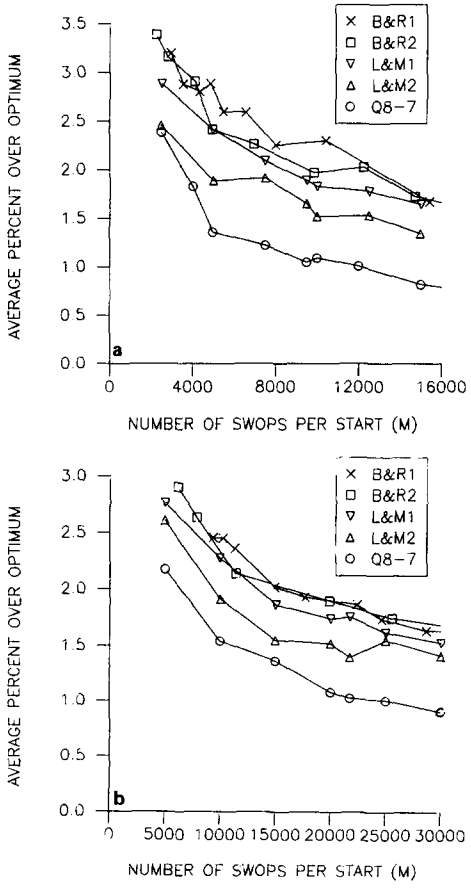

Figure 3. (a) %deviation averaged over 100 trials on NUG20. (b) %deviation averaged over 100 trials on NUG30

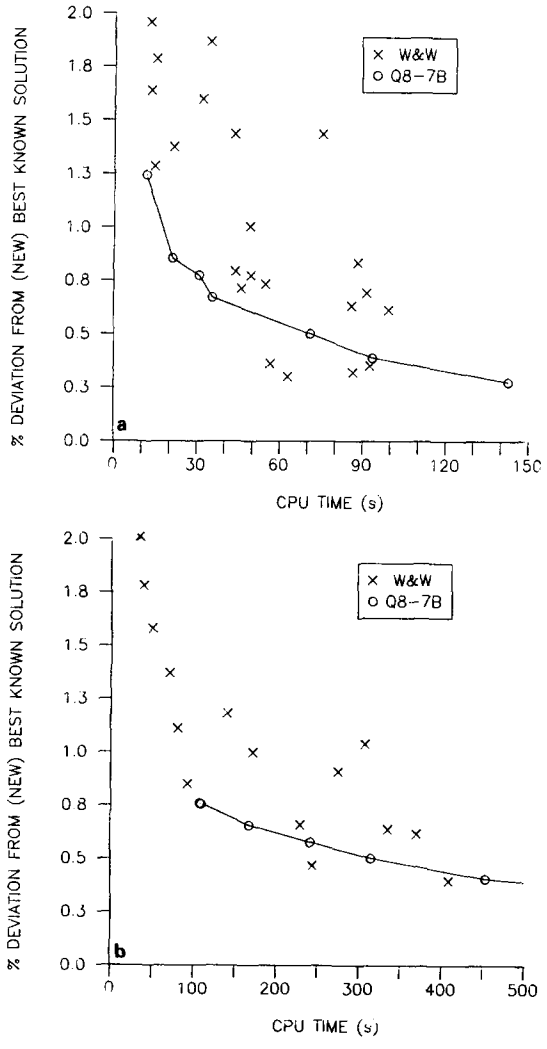

Figure 4. (a) W&W vs. Q8-7B on W&W50. (b) W&W vs. Q8-7B on W&W100

These two annealing schemes, along with the three schemes L&M1, L&M2 and Q8-7 described above were run 100 times on the two largest Nugent et al. problems ($n = 20$ and 30), and the average percentage deviation from the best known solutions (2570 and 6124 respectively) are illustrated graphically in Figure 3. It is clear that Q8-7 is superior to the other four schemes implemented by the author, achieving anything up to a 50% reduction in the number of swops required to achieve a given performance level. (Note that all the schemes required approximately the same amount of CPU time to examine a specified number of potential swops.)

In [16] Wilhelm and Ward report on the use of another annealing scheme which involves waiting for convergence at each temperature before cooling to the next. They give a large number of results for a variety of parameter settings. Their results for the two largest problems ($n = 50$ and 100) (modified to take account of the improved best known solutions) are plotted in Figure 4, along with the results of running Q8-7B with a range of values for M and default values for the other parameters. Note that this comparison assumes the equivalence of the "DEC KL 1059 mainframe" used by Wilhelm and Ward, and the Vax 11/785 used by this author. If this is a valid assumption then clearly Q8-7B is performing well compared with the more complicated and parameter-sensitive scheme used in [16]—A conclusion backed up by the improved solutions found by the Q8-7B algorithm.

Conclusions

The main conclusions of this paper are as follows:

(i) Simulated annealing is an extremely efficient heuristic for the QAP.

(ii) For this problem a sequential generation of neighbours is superior to a random selection method in an annealing scheme.

(iii) There exists a fixed temperature at which the performance of an annealing scheme is optimised.

(iv) A scheme incorporating these ideas has been written which performs extremely well, finding improved solutions for several of the largest problems in the literature in only modest amounts of CPU time without the need to 'tune' the system for each new data set. The resulting algorithm must be considered to be one of the most effective heuristics available for this notoriously difficult class of problem.

Acknowledgement

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