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## Neural Networks

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Preface

reflected in the acceptance ratio, which was only about 40% the selection of the full contributions was performed by an international were placed on the origin of the participants in this workshop. Instead European Association for Signal Processing, EURASIP), no restrictions EURASIP Workshop on Neural Networks, held in Sesimbra, Portugal February 15-17, 1990. Though sponsored by a European organization (the This book contains both the full and the invited contributions to Committee. The quality demands that were imposed

overspecialized topic: one main characteristic of nonlinear models suggested by nature. Authors of this book belong to all been studied previously by computer scientists, and engineers may essential features of the world these disciplines pertorm community is field schemes, biologists can describe architectures that have not simulations and implementations of connectionist architectures, help of mathematicians is most welcome to of its multidisciplinarity. Psychologists may identify the the contributions to be learned and propose original has not been the restricted formalize these connectionist to

approached with an engineering methodology, instead of the present trialand-error manner embryo of a body of theory that will allow neural network problems to be and generalization capability. We can only hope that these will form the relevant to neural networks and discusses some of its properties. Eric study of the capabilities of neural networks. George Cybenko introduces we consider very important for the consolidation of the field: Baum studies the relationships between training set size, network size the definition of special mention. They deal with two different aspects of a subject which two invited papers, by George Cybenko and by Eric Baum, deserve a a formal measure of problem complexity which is the formal

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# IMPROVED SIMULATED ANNEALING, BOLTZMANN MACHINE, AND ATTRIBUTED GRAPH MATCHING †

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Abstract. By separating the search control and the solution updating of the commonly used simulated annealing technique, we propose a revised version of the simulated annealing method which produces better solutions and can reduce the computation time. We also use it to improve the performance of the Boltzmann machine. Furthermore, we present a simple combinatorial optimization model for solving the attributed graph matching problem of e.g. computer vision and give two algorithms to solve the model, one using our improved simulated annealing method directly, the other using it via the Boltzmann machine. Computer simulations have been conducted on the model using both the revised and the original simulated annealing and the Boltzmann machine. The advantages of our revised methods are shown by the results.

1. Introduction. Simulated Annealing (SA) has been widely used to solve various combinatorial optimization problems such as TSP, VLSI design [1,2] as well as clustering and attributed graph matching [3]. It has also been used in the Boltzmann Machine (BM) [4, 5-7].

By separating the Metropolis Sampling (MS) process which is a major part of the SA process, into a search control process and a solution updating process, one of the present authors proposed an Improved Simulated Annealing (ISA) method [8,9] which will be reviewed and further analyzed in this paper. This method can be guaranteed to always yield a better solution than SA. It is useful especially in the following cases, which are often encountered in actual applications:

(1) The time spent on each MS process is not long enough to let the process reach the equilibrium state.

(2) The speed of annealing is too fast.

\* (3) The temperature specified for stopping the annealing process is not low enough. In these cases, SA usually finds a bad solution, but ISA can still obtain a better solution. In addition, ISA also has a simple but effective way to decide when a MS process can be finished to start another MS process, and when the whole annealing process can be stopped in such a way that the time cost is reduced but the solution is still satisfactory.

Furthermore, in this paper we will use the basic idea of ISA to improve the performance of BM. Advantages similar to the ones given above are again obtained.

Our work is motivated by the computer vision problem. Attributed graphs have turned out to be very useful data structures when used for image representation and understanding in computer vision systems [10-12]. They have also been successfully

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used to handle optimal task assignments in distributed computer systems [13]. In [3], one of the authors proposed a way to use SA to implement attributed graph matching. This paper will give another solution: a general attributed graph matching problem is turned into a model of combinatorial optimization which is different from that in [3]. With this model, we can either directly use SA or use symmetrically interconnected neural networks via the BM to obtain the solution of attributed graph matching.

In sec. 2, the commonly used SA algorithm is analyzed. In sec. 3, the ISA is given, its advantages are discussed, and it is applied on the BM. In sec. 4, a general combinatorial optimization model for attributed graph matching is presented and solved by ISA and the revised BM. Finally, in sec. 5, the advantages of ISA are shown through computer simulations with performance comparisons on both the optimality of solution

2. Analysis of Simulated Annealing. In problem-solving with SA, each combinatorial state  $s_i$  is regarded as a configuration state of a physical system, the objective function  $E(s_i)$  as the system energy, and a parameter T is used to imitate temperature. For a given T, MS is used to simulate the thermodynamical equilibrium at which the Boltzmann distribution  $E(s_i)$ 

$$f(s_i) = \frac{e^{-E(s_i)}}{\sum_i e^{-E(s_i)}} \tag{1}$$

can properly describe the probability of the energy at each state. As T gradually decreases,  $f(s_i)$  becomes sharp around the state of global minimum energy and will be fixed at the state as  $T \to 0$ , i.e., the global optimization solution can be obtained.

Generally, the commonly used SA could be described as follows:

Initialization: Generate a random state s as the present solution, and initialize E(s) and  $T = T^{(0)}$ ;

step 1: Randomly make a small perturbation  $\Delta s$  to get a new state  $s + \Delta s$  with the energy increment  $\Delta E = E(s + \Delta s) - E(s)$ ;

step 2: If  $\Delta E < 0$  goto step 3, otherwise, generate a random number  $\xi$  by sampling a uniform distribution over [0,1] and if  $e^{-\Delta E/T} \leq \xi$ , goto step 1;

step 3:  $s + \Delta s$  replaces s as the new present solution, and  $E := E + \Delta E$ ;

step 4: Check whether the MS at the present T reached its equilibrium; if not, goto step 1:

step 5: Reduce T into T' < T by some means (e.g.,  $T := \lambda T$ ). Check whether the annealing process has terminated (e.g.,  $T < T_{min}$ ); if yes, the present s with its E(s) is taken as the final solution, stop; otherwise, goto step 1.

There steps 1,2,3,4 implement the MS process and step 5 imitates the annealing procedure. The effectiveness of SA depends on: (1) Whether each MS process reaches its equilibrium, i.e., how long each MS process should take at each T. (2) Whether  $T^{(0)}$  is high enough,  $T_{min}$  is low enough. and T decreases slowly enough. A low  $T^{(0)}$  high  $T_{min}$ , sharply decreasing T and short time implementation for each MS process will lead to low computer cost, but the solution is not so good. In contrast, very high  $T^{(0)}$ , very low  $T_{min}$ , and slowly decreasing T will always result in an optimal or nearoptimal solution, but usually the cost is substantially high. Although there are several

investigations (including some theoretical analysis) on how to select the above paters, they are either preliminary or theoretical. The common way is still simply to  $T^{(0)}, T_{min}$ , a fixed number of steps for each MS process in a heuristic way, and decrease exponentially by  $T := \lambda T(0 < \lambda < 1)$  [1][7].

The above procedure contains a drawback related to the sequence of solution  $s_{i,j}$  denote the present solution of the j-th iteration at  $T_i$ , one iteration being one from step 1 to step 5. Then all the present solutions produced during the implement of SA will form an updating sequence  $\{(s_{i,j}, j = 0, 1, ...), i = 0, 1, ...\}$ . The secretords the updating history of the present solution, as well as of the track that how the search is controlled. The relation between  $s_{i,j}$  and  $s_{i,j+1}$  has three possible  $S_i$  and  $S_i$  are the possible sequence of the present solution at  $S_i$  and  $S_i$  and  $S_i$  and  $S_i$  are the present solution at  $S_i$  and  $S_i$  and  $S_i$  are the present solution at  $S_i$  and  $S_i$  and  $S_i$  and  $S_i$  are the present solution at  $S_i$  and  $S_i$  are the present solution at

(a).  $E(s_{i,j+1}) < E(s_{i,j})$ , if  $\Delta E < 0$  in step 2

(b).  $E(s_{i,j+1}) > E(s_{i,j})$ , if  $\Delta E > 0$  and  $e^{-\Delta E/T_i} > \xi$  in step 2. (c).  $E(s_{i,j+1}) = E(s_{i,j})$ , if  $\Delta E > 0$  and  $e^{-\Delta E/T_i} \le \xi$  in step 2.

Obviously,  $\{(E(s_{i,j}), j=0,1,\ldots), i=0,1,\ldots\}$  is not a monotonically unincresquence.

Possibility (b) allows the present solution to escape from local minima. If the key point of the MS process in SA. But it also allows the possibility that the solution  $E(s_{q,p})$  (suppose SA stopped after p steps at  $T_q$ ) may be worse than earlier solutions  $E(s_{i,j}), j < p, i < q$ . This may happen especially if the replacen  $T_i$  by  $T_{i+1}$  occurs before the MS process at  $T_i$  reaches its equilibrium, or  $T^{(0)}$  high enough and  $T_{min}$  not low enough, or T decreases too fast. As stated in sec.1 cases are often encountered in practice since there is still no appropriate way to these parameters.

The above analysis explains why the solution by simulated annealing is som even worse than that by some conventional heuristic methods, and it also explain curve phenomenon in Fig.7d in ref. [2].

3. ISA and a Related Improvement on BM. Although necessary for the control to escape from local minima, possibility (b) above impacts a bad influe the updating sequence of the present solution. The contradiction can be solve separating the search track and the updating sequence of the present solution. We retain  $\{(s_{i,j}, j=0,1,\ldots), i=0,1,\ldots\}$  as the search track, and construct a new sets, as the updating sequence of the present solution:

$$\hat{s}_{0,0} = s_{0,0}; if \ E(s_{i,j+1}) < E(s_{i,j}) \ then \ \hat{s}_{i,j+1} = s_{i,j}; \ otherwise \ \hat{s}_{i,j+1} = s_{i,j};$$

and if  $s_{i,k}$  is the last state at  $T_i$  and  $s_{i+1,0}$  is the first state at  $T_i$ , then

if 
$$E(s_{i+1,0}) < E(s_{i,k})$$
 then  $\hat{s}_{i+1,0} = s_{i,k}$ ; otherwise  $\hat{s}_{i+1,0} = \hat{s}_{i,k}$ .

This modification results in ISA which has the following three advantages:

(1). All the good features of SA can be retained (since the search track changed), but a better final solution can be obtained since  $\{(E(\hat{s}_{i,j}), j=0,1,...)\}$  is now monotonically unincreasing.

(2). At a given  $T_i$ , if in q successive states  $\hat{s}_{i,j} = \hat{s}_{i,j+1} = \dots = \hat{s}_{i,j+q}$  hold q is large enough, it could be considered that the equilibrium has been approximately

reached. So, a simple and effective way to check whether MS process could be stopped at temperature  $T_i$  is to check whether  $q>q_0$  (a given threshold).

(3). Let  $\hat{s}_{i,k_i}$  denote the last present solution at  $T_i$ . If in p successive temperatures  $\hat{s}_{i,k_i} = \hat{s}_{i+1,k_{i+1}} = \ldots = \hat{s}_{i+p,k_{i+p}}$  holds, and p is large enough, it could be considered that any further reduction of T is useless. So, a way to check whether the whole annealing process could be stopped is to check whether  $p > p_0$  (a given threshold).

The first advantage makes the solution obtained by ISA better than that obtained by SA at nearly the same computing cost. The last two advantages can considerably reduce the computing cost but still keep a good solution.

The algorithm for implementing ISA is given as follows:

Initialization: Generate a random state s as the present solution, and initialize E(s) and  $T = T^{(0)}$ ; set  $T_{min}$ ,  $j_{max}$ ,  $q_0$ ,  $p_0$ ; Let p = 0, q = 0, j = 0,  $\hat{s} = s$ , E = E(s),

 $E_{\hat{s}} = E$ ,  $E_t = E$ ; step 1: If  $j > j_{max}$ , goto step 6; otherwise, j := j + 1, randomly make a small perturbation  $\Delta s$  to get a new state  $s + \Delta s$  with the energy increment  $\Delta E = E(s + \Delta s) - E(s)$ ;

step 2: If  $\Delta E > 0$ , generate a random number  $\xi$  by sampling a uniform distribution over [0,1]. If  $e^{-\Delta E/T} \leq \xi$ , goto step 1;

step 3:  $s+\Delta s$  replaces s as the new present solution, and  $E:=E+\Delta E;$  step 4: If  $E< E_{\hat{s}}$  then  $E_{\hat{s}}:=E$  and  $\hat{s}:=s+\Delta s$ , q:=0; Otherwise q:=q+1;

step 5: If  $q < q_0$ , goto step 1;

step 6: If  $E_t < E_s$  then  $E_t := E_s$  and p := 0; Otherwise p := p + 1;

step 7: If  $p < p_0$  and  $T > T_{min}$ , reduce T into T' < T by some means(e.g., $T := \lambda T$ ), q := 0 and k := 0 and goto step 1; Otherwise, the present  $\hat{s}$  with its  $E(\hat{s})$  is taken as the final solution, stop.

There  $T_{min,j_{max}}$ , respectively, are given thresholds for the minimum temperature and for the maximum time of the MS process at each  $T_i$ . The two thresholds together with  $q_0$  and  $p_0$  control when the MS process at each  $T_i$  finishes and when the whole annealing stops.

The same method can be applied to the BM in a straightforward way. The BM is a symmetrical interconnected neural network with energy expression:

$$E = -0.5 \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} c_i c_j + \sum_{i=1}^{n} \theta_i c_i$$
 (3a)

where  $\theta_i$  is a threshold associated to neuron  $c_i$ . The basic solution step is as follows: At a given T, select a neuron  $c_i$ , calculate its energy gap  $\Delta E_i$  (i.e., the difference between the energy of the two global states, one with neuron  $c_i$  off ( $c_i = 0$ ) and the other with neuron  $c_i$  on ( $c_i = 1$ )) by

$$\Delta E_i = \sum_{i=1, j \neq i}^{n} w_{ij} c_j - \theta_i \tag{3b}$$

and let the neuron  $c_i$  take the value  $c_i = 1$  with probabilty

$$p_i = 1/(1 + exp(-\Delta E_i/T)).$$

(4)

Then, select another neuron and repeat the same process until the equilibrium is re. The whole process starts at a high temperature T, and gradually decreases T on equilibrium is reached, until a low enough T value is reached.

The BM can be revised in a similar way as SA in sec. 3. What we need is to also set up a new updating sequence of the present solutions. This can be as follows: In addition to a binary array A which indicates the current global state network, another binary array B is used to record the global state of the cominimal energy. Initially, both arrays A = B record a randomly chosen global. Then A will be updated once each neuron  $c_i$  changes its value according to probab given by Eq.(4), but B is updated by B = A only when the energy of the current state is lower than the energy of the state recorded in B. In this way, a monoto unincreasing energy sequence of the current solution is obtained. When the process is stopped, the current state recorded in B could be taken as the final so

4. Attributed Graph Matching by ISA and the Improved BM. Attr Graphs have shown superior adequacy when used for image representation and standing in computer vision [10-12]. They have also been successfully used e handle optimal task assignment in distributed computer systems [13].

To fix the notation, assume an attributed graph  $G = [(V, V_a), (E, E_a)]$ .  $V = (v_1, v_2, ..., v_n)$  is the node (vertex) set and  $V_a = (av_1, av_2, ..., av_n)$  its not tribute set, and  $E = (e_1, e_2, ..., e_p)$  is the edge set and  $E_a = (ae_1, ae_2, ..., ae_p)$  it attribute set. Both for nodes and edges, each attribute may be either a symbolical merical variable. The problem of matching two attributed graphs,  $G = [(V, V_a), (I_a)]$  and  $G' = [(V', V'_a), (E', E'_a)]$  with node sets  $V = (v_1, v_2, ..., v_n)$ ,  $V' = (v'_1, v'_2, ..., v_n)$  means setting up a one-to-one correspondence between the nodes of a subset of G'. Generally speaking, there will be m!/(m-n)! (assume  $m \geq n$ ) combinationstructing one-to-one correspondences between nodes of a subset of G and G'. ically, when n = m the problem is called attributed graph matching; when n < 0 problem is called attributed subgraph matching.

Usually, there is some cost associated with constructing a one-to-one corredence between a node  $v \in V$  and a node  $v' \in V'$  and between an edge  $e \in E$ : edge  $e' \in E'$ ; denote the costs by d(v,v') and d(e,e') respectively. Specifically, d(e,e') can be calculated from the differences between the attributes of v and and e'). e.g, for numerical attributes, d(v,v') may be the square distance betwee attributes of v and v'. Thus, for each combination, we can sum up all the d(v,v') deget a total cost D(G,G'). The goal of attributed graph matching is to among all the possible combinations one that has the minimum value of D(G,G') the optimal match between G and G', or a near minimal value of D(G,G') for match between G and G'.

To form the objective function in practice, define a binary  $n \times m$  matrix [1] which each row i corresponds to a node  $v_i$  of G and each column j correspondence  $v_i'$  of G'. If a one-to-one correspondence is assigned to a pair of nodes  $v_i$ , v element  $U_{ij} = 1$ , otherwise  $U_{ij} = 0$ . For a feasible matching possibility, the sur elements  $U_{ij}$  equals n (here, suppose  $n \le m$ ), and there should be one and or element  $U_{ij} = 1$  in each row and at most one element  $U_{ij} = 1$  in each column.

when n = m. The value of the whole matrix is considered as a combinatorial state. there should be one and only one element  $U_{ij} = 1$  both in each row and each column

torial states choose one which makes the following objective function take the minimal A combinatorial optimization model is proposed as follows: among all the combina-

(i) For n = m

$$E = a \sum_{i=1}^{n} \left( \sum_{j=1}^{n} U_{ij} - 1 \right)^{2} + a \sum_{j=1}^{n} \left( \sum_{i=1}^{n} U_{ij} - 1 \right)^{2}$$

$$+b\sum_{i=1}^{n}\sum_{j=1}^{n}(av_{i}-av_{j}^{l})^{2}U_{ij}+c\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{l=1,l\neq i}^{n}\sum_{k=1,k\neq j}^{n}(ae_{ij}-ae_{lk}^{l})^{2}U_{i}U_{jk}^{l}$$

(5a)

(ii) For n < m</p>

$$E = a \sum_{i=1}^{n} (\sum_{j=1}^{m} U_{ij} - 1)^{2} + a (\sum_{j=1}^{n} \sum_{i=1}^{m} U_{ij} - n)^{2}$$

$$+b\sum_{i=1}^{n}\sum_{j=1}^{m}(av_{i}-av'_{j})^{2}U_{ij}+c\sum_{i=1}^{n}\sum_{j=1}^{m}\sum_{l=1,l\neq i}^{n}\sum_{k=1,k\neq j}^{m}(ae_{ij}-ae'_{lk})^{2}U_{i}U_{jk}$$
(5b)

of G and V' of G'. The 3rd and 4th terms attempt to minimize the total costs of all is now possible to use the SA or ISA to minimize these objective functions. d(v,v') and d(e,e'), respectively. The coefficients a, b, and c are weight parameters. It tively. The first two terms attempt to insure a one-to-one correspondence between V where  $ae_{il}, ae'_{jk}$  denote the attribute vectors of the edges  $e(v_i, v_l)$  and  $e(v'_j, v'_k)$ , respec-

of randomly inversing an element  $U_{ij}$  into  $U_{ij} := 1 - U_{ij}$  and then locally calculating energy increment  $\Delta E$ . For the model of Eq.(5), we treat the two tasks in a simple way to solve the graph matching problem are how to perturb the present state (i.e, from its resulted  $\Delta E$  by present state s to a new state  $s + \Delta s$ ) and how to locally calculate the corresponding As one of the present authors pointed out in [3], the two key points in using SA

$$\Delta E(U_{ij}, 0 \to 1) = 2a \sum_{k=1, k \neq j}^{n} U_{ik} + 2a \sum_{k=1, k \neq i}^{n} U_{kj} - 2a$$

$$+b(av_i - av'_j)^2 + 2c \sum_{r=1, r \neq i}^{n} \sum_{q=1, q \neq j}^{m} (ae_{ri} - ae'_{qj})^2 U_{rq}$$

and 
$$\Delta E(U_{ij}, 1 \to 0) = -\Delta E(U_{ij}, 0 \to 1)$$
  
(ii) For  $n < m$ 

$$\Delta E(U_{ij}, 0 \to 1) = 2a \sum_{k=1, k \neq j}^{n} U_{ik} + 2a \sum_{r=1, r \neq i}^{n} \sum_{q=1, q \neq j}^{m} U_{rq} - 2a\mathbf{T}$$

$$+b(av_i-av_j')^2+2c\sum_{r=1,r\neq i}^{n}\sum_{q=1,q\neq j}^{m}(ae_{ri}-ae_{qj}')U_{rq}$$

and  $\Delta E(U_{ij}, 1 \to 0) = -\Delta E(U_{ij}, 0 \to 1)$ 

are obtained directly for solving the model of Eq.(5): By using the procedures of SA and ISA proposed in sec. 3, the following algori

### Algorithm AGM-SA

Initialization: Set an  $N \times M$  Matrix  $[U_{ij}]$  by randomly deciding each of its element be 1 or 0; initialize E by Eq.(5), and  $T = T^{(0)}$ ; set  $T_{min}$ ,  $k_{max}$ ; let k = 0;

step 1: If  $k > k_{max}$  goto step 4; k := k + 1; Choose with equal probabiliti by Eq.(6); integer i among [1,2,...,N] and an integer j among [1,2,...,M]; Comput

If  $exp[-\Delta E/T]$ )  $\leq \xi$  goto step 1; step 3:  $U_{ij} := 1 - U_{ij}$  and  $E := E + \Delta E$ ; step 2: Generate a random number \( \) by sampling a uniform distribution over

step 4: If  $T > T_{min}$  then  $T := \lambda T$  (0 <  $\lambda$  < 1) and k := 0 and goto step 1; other the present  $[U_{ij}]$  with value E is taken as the final solution and stop.

### Algorithm AGM-ISA

 $T^{(0)}$ ,  $T_{min}$ ,  $k_{max}$ ,  $q_{max}$ ,  $p_{max}$ ; Let p = 0, q = 0, k = 0,  $\hat{s} = s$ , E = E(s),  $E_{\hat{s}}$ be 1 or 0, and let another  $N \times M$  Matrix  $[U'_{ij}]$  take the same values as  $[U_{ij}]$ ; Init Initialization: Set an  $N \times M$  Matrix  $[U_{ij}]$  by randomly deciding each of its element

step 1: k := k+1; Choose with equal probabilities an integer i among [1,2,...,N]an integer j among [1,2,...,M]; Compute  $\Delta E$  by Eq.(6);

step 2: If  $\Delta E < 0$  goto step 4, otherwise, generate a random number  $\xi$  by same a uniform distribution over [0,1]; If  $exp[-\Delta E/T]$ ) >  $\xi$  goto step 4;

step 4:  $U_{ij} := 1 - U_{ij}$  and  $E := E + \Delta E$ ; step 3: If  $k > k_{max}$ , goto step 7, otherwise goto step 1;

step 5: If  $E < E_{\mathfrak{z}}$  then  $E_{\mathfrak{z}} := E$  and  $[U'_{ij}] := [U_{ij}]$  and q := 0; Otherwise q := q

step 6: If  $q < q_{max}$ , goto step 1;

step 7: If  $E_t \gg E_s$  then  $E_t := E_s$  and p := 0; Otherwise p := p + 1;

step 8 : If  $p < p_{max}$  and  $T > T_{min}$  then  $T := \lambda T$   $(0 < \lambda < 1)$ and q := 0 and k = 0and goto step 1; Otherwise, the present  $[U'_{ij}]$  is taken as the final solu and use Eq.(5) to calculate its E and stop.

be further rewritten into the following form: When we wish to solve the same problem with BM or Improved BM, Eq. (5

(6a)

$$\begin{split} E &= -0.5 \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{l=1}^{n} \sum_{k=1}^{m} w_{ij,lk} U_{ij} U_{lk} - \sum_{i=1}^{n} \sum_{j=1}^{n} U_{ij} \theta_{ij}, \\ w_{ij,lk} &= -2a(\delta_{il} + \delta_{jk}) - 2c(1 - \delta_{il})(1 - \delta_{jk})(ae_{ij} - ae'_{lk})^2, \\ \theta_{ij} &= -4a + b(av_i - av'_j)^2 \end{split}$$

where  $\delta_{ij}$  is the Kronecker delta;

$$\begin{split} E &= -0.5 \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{l=1}^{n} \sum_{k=1}^{m} w_{ij,lk} U_{ij} U_{lk} - \sum_{i=1}^{n} \sum_{j=1}^{m} U_{ij} \theta_{ij}, \\ w_{ij,lk} &= -2a(\delta_{il} + 1) - 2c(1 - \delta_{il})(1 - \delta_{jk})(ae_{ij} - ae'_{lk})^2, \\ \theta_{ij} &= -2a(n+1) + b(av_i - av'_j)^2. \end{split}$$

then matrix  $[U_{ij}]$  constitutes a symmetrically interconnected neural network that BM  $w_{ij,lk} = w_{lk,ij}$ , i.e.,  $w_{ij} = w_{ji}$ . Therefore, if each element  $U_{ij}$  is regarded as a neuron and if the distance function  $d(\cdot,\cdot)$  satisfies d(x,y)=d(y,x), then it is easy to see that and  $\theta_{ij}$  to  $\theta_i$ . If the edges of G and G' are undirectional, i.e.,  $e_{il} = e_{li}$  and  $e'_{jk} = e'_{kj}$  $U_{ij}, U_{lk}$  correspond to neurons  $s_i, s_j$ , respectively,  $w_{ij,lk}$  corresponds to connections  $w_{ij}$ , Compare Eq.(7) with the energy expression Eq.(3); it is not difficult to see that

of Eq.(5). Due to the limited space, we do not here introduce the details which can be As a result, BM and The improved BM can also be directly used to solve the model

define  $d(e_{ij}, e_{ij}^t) = 0$ . These costs are used for computing the total matching cost E by Eq.(5) and  $\Delta E$  by Eq.(6). In these formulas, the parameters are a = 1000.0, b = 1.0 $e_{ij}$   $(e'_{ij})$ , for edges  $e_{ij} = e(v_i, v_j)$ ,  $e'_{ij} = e(v'_i, v'_j)$ . Specifically, for  $e_{ij}$ ,  $e'_{ij}$ , if one is a where  $av_i(av'_j)$  is the attribute of node  $v_i(v'_j)$  and  $ae_{ij}(ae'_{ij})$  is the attribute of edge corresponding attributes, i.e.,  $d(v_i, v_j') = (av_i - av_j)^2$  and  $d(e_{ij}, e_{ij}') = (ae_{ij} - ae_{ij}')^2$ of nodes (edges) between G and G' are defined by the square distance between their structure as G, but its node labels are all wrong. The cost of one-to-one correspondence digit and each edge attribute is denoted by a circled digit. G' has the same topological On each node and edge there is an attribute. Each node attribute is denoted by a in Fig.1. There are two attributed graphs G, G', each having 8 nodes and 10 edges 5. Computer Simulations. One of our attributed graph matching problems is shown define  $d(e_{ij}, e'_{ij}) = 10^6$  to penalize the correspondence; but if both are pseudo-edges, we pseudo-edge (i.e., there is no real edge between the two nodes) and the other is not, we

still kept the other parameters unchanged, but continuosly reduced Tmin to 1.0. After as given in Fig.2(c), but with the extra cost of 38077 perturbations. Hereafter, we the algorithm stopped at  $T=9.644 < T_{min}$ . The global solution E=0.5 was obtained other parameters unchanged, but decreased Tmin to 10.0. After 52105 peturbations solution E=3010.25 is bad and not feasible as shown in Fig.2(b). Then we kept the pointed out in sec.2.2, the solution mistakenly jumped from the optimal one to an 74649 perturbations, the algorithm stopped at T=0.9591. However, due the drawback (1) First, AGM-SA was used. For a group of parameters T=2000,  $T_{min}=500$ ,  $k_{max}=500$ , and  $\lambda=0.95$ , the initial match was randomly generated as given in unfeasible one with E=1025.5. Then as we continued to lower  $T_{min}$ , the solution (iterations), the algorithm stopped since the present  $T=475.65 < T_{min}$ . The final Fig.2a, which is a very bad match and totally unfeasible. After 14028 perturbations

> optimality of the solution. that for AGM-SA, Tmin not only greatly influences the time cost but also influe still a bad and unfeasible one, as given in Fig.2(d). These experiments also never returned to the optimal one; even after 119194 perturbations, the so

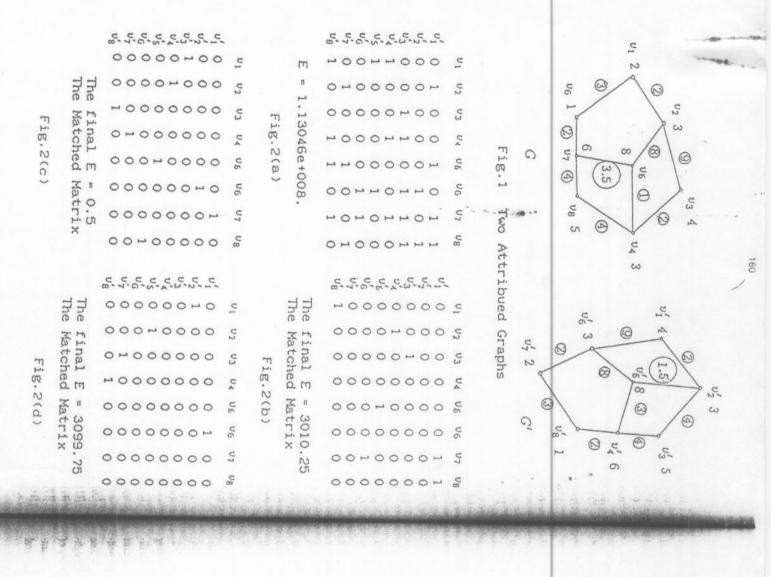
condition and the initial match) and the same group of parameters as those in only 7384 perturbations. The global optimal solution was still obtained  $p_{max} = 15$ , but kept all the other parameters unchanged. The algorithm stopp will never be lost by further lowering  $T_{min}$ . In another trial, we let  $q_{max}$  = perturbations saved) and the optimality of solution. Forthermore, the optimal perturbations, the algorithm stopped at the global optimal solution as given ir ment (1) were used. In the first trial with  $q_{max} = +\infty$  and  $p_{max} = +\infty$ , also after (2) Second, AGM-ISA was used. The same conditions (including the ran This is obviously better than that obtained by AGM-SA both in the time cos

in SA has been separated by constructing a new present solution updating so and the computing cost. We have also shown that a similar improvement can As a result, an improvement has been made to SA, on both the optimality of 6. Summary. The search track and the updating sequence of the present

of a combinatorial optimization problem, SA and BM as well as their correspon over their original forms were shown through computer simulations with perf proved versions were used to solve the model. The advantages of the improved comparisons on both the optimality of solution and the time cost After modeling the attributed graph matching problem by the objective

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