

# A deterministic annealing algorithm for a combinatorial optimization problem using replicator equations

Kazuo Tsuchiya\*, Takehiro Nishiyama, Katsuyoshi Tsujita

*Department of Aeronautics and Astronautics, Graduate School of Engineering, Kyoto University, Kyoto 606-8501, Japan*

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## Abstract

We have proposed an optimization method for a combinatorial optimization problem using replicator equations. To improve the solution further, a deterministic annealing algorithm may be applied. During the annealing process, bifurcations of equilibrium solutions will occur and affect the performance of the deterministic annealing algorithm. In this paper, the bifurcation structure of the proposed model is analyzed in detail. It is shown that only pitchfork bifurcations occur in the annealing process, and the solution obtained by the annealing is the branch uniquely connected with the uniform solution. It is also shown experimentally that in many cases, this solution corresponds to a good approximate solution of the optimization problem. Based on the results, a deterministic annealing algorithm is proposed and applied to the quadratic assignment problem to verify its performance. © 2001 Elsevier Science B.V. All rights reserved.

*Keywords:* Combinatorial optimization problem; Replicator equation; Bifurcation; Deterministic annealing algorithm

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## 1. Introduction

A combinatorial optimization problem is an optimization problem in which decision variables are discrete. The quadratic assignment problem (QAP) [1] is a typical instance of this class of optimization problem. The QAP is a problem to minimize the performance index defined as a quadratic function of the decision variables under some constraints. For the QAP, a variety of approximation methods have been proposed. Among them, there is a dynamical systems approach. One of the models of this approach is the Hopfield model [2]. The Hopfield model is derived as the mean field theory approximation of an Ising model [3]. The model is composed of the elements with the input–output characteristics expressed by a sigmoid function, and derived as the gradient vector field of the potential function composed of the performance index and the constraints. When the slope of the sigmoid function is large, the elements take binary states. As a result, an approximate solution of the optimization problem is obtained as a stable equilibrium solution of the system. In order to improve the solution, the deterministic annealing is applied [4]; the slope of the sigmoid function is increased gradually so that a good local minimum solution is obtained. A model which is derived as the mean field theory approximation of a Potts model has been proposed [5]. A Potts model is a generalization of an Ising model so as to take more than two states. By employing a Potts model, some

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\* Corresponding author.

of the constraints are to hold automatically. Furthermore, based on a Potts model, the models which satisfy all the constraints except for the binary constraints automatically have been proposed, i.e. doubly constrained network by Ishii and Sato [6] and soft-assign by Rangarajan et al. [7]. On the other hand, a model based on the  $\lambda$ -opt heuristics has been proposed, i.e. the  $\lambda$ -doubly constrained network by Ishii and Niitsuma [8].

We have proposed a model based on replicator equations [9,10].<sup>1</sup> The replicator equation is the equation where the derivatives of variables are proportional to the states of the variables. The proportionality coefficients are called the growth rates. The growth rates of the model are composed of the performance index and the constraints. We revealed the following stability characteristics of the equilibrium solutions of the model. (1) In the region where a parameter in the growth rates is small, only one equilibrium solution, the uniform solution, is stable whereas in the region where the parameter is large, only the equilibrium solutions which satisfy the constraints, the feasible solutions, are stable. (2) When the parameter is increased, the feasible solutions become stable approximately in the order, from the one having the smallest performance index to the largest one. Based on the results, we have proposed a deterministic annealing algorithm. But, during the annealing process, bifurcations occur and affect the performance of the algorithm. The analysis of the bifurcation characteristics has not been sufficiently carried out. In this paper, the bifurcation characteristics are analyzed and based on the results, a new deterministic annealing algorithm is proposed.

First, in Section 2, the QAP is introduced and in Section 3, equilibrium solutions of the proposed model and their stabilities are mentioned briefly. In Section 4, the bifurcation characteristics of the proposed model are analyzed. Based on the analysis, a deterministic annealing algorithm is proposed in Section 5, and the algorithm is applied to many instances of the QAP to verify the performance of the algorithm in Section 6. Finally, we briefly summarize the results in Section 7.

## 2. The quadratic assignment problem

The QAP [1] is defined as follows:

$$\min_{p \in \Pi_{\mathcal{N}}} L(p), \quad (1)$$

$$L(p) = \sum_{i,j} a_{ij} b_{p(i)p(j)}, \quad (2)$$

where  $A = a_{ij}$  and  $B = b_{kl}$  are  $N \times N$  matrices,  $\Pi_{\mathcal{N}}$  is the set of all permutations of  $\mathcal{N} = \{1, \dots, N\}$  and  $p$  an element of  $\Pi_{\mathcal{N}}$ . Using permutation matrices, the QAP can also be stated as follows:

$$\min_{X \in \Pi_{N \times N}} L(x_{ij}), \quad (3)$$

$$L(x_{ij}) = \text{trace}(A^T X^T B X) = \sum_{i,i',j,j'} a_{ij'} b_{i'j} x_{ij} x_{i'j'}, \quad (4)$$

where  $\Pi_{N \times N}$  is the set of all  $N \times N$  permutation matrices and  $X = x_{ij}$  an element of  $\Pi_{N \times N}$ .

The QAP is considered one of the hardest combinatorial optimization problems. For a QAP, the number of feasible solutions is  $N!$  and it increases explosively with  $N$ . Therefore, it is practically impossible to compute values of the

<sup>1</sup> Recently, Haken et al. [11,12] have proposed a model for a combinatorial optimization problem based on replicator equations (they use the term ‘‘coupled selection equation’’ instead of the term ‘‘replicator equation’’). However, their model is for a linear assignment problem and does not apply to the QAP directly, so we do not refer the model here.

performance index for all these solutions, and heuristic algorithms are needed to obtain good approximate solutions in relatively short time.

### 3. Equilibrium solution of the proposed model and its stability [9,10]

In this section, we briefly explain the proposed model and its characteristics. The model is given as a following replicator equation:

$$\dot{u}_{ij} = f_{ij}(u_{i'j'}, \alpha_0, \alpha_1)u_{ij}, \tag{5a}$$

$$f_{ij} = (1 - u_{ij}^2) - \frac{\alpha_0}{2} \left( \sum_{i' \neq i} u_{i'j}^2 + \sum_{j' \neq j} u_{ij'}^2 \right) - \frac{\alpha_1}{2} \sum_{i',j'} (a_{ij'}b_{i'i} + a_{j'j}b_{i'i})u_{i'j'}^2, \quad i, j = 1, \dots, N, \tag{5b}$$

where the variable  $u_{ij}$  ( $i, j = 1, \dots, N$ ) expresses the  $(i, j)$ th element of an  $N \times N$  matrix, and parameters are  $\alpha_0 > 0$  and  $0 \leq \alpha_1 \ll 1$ . The first term of the right-hand side of Eqs. (5a) and (5b) leads each  $u_{ij}^2$  to unity. The second term represents the effect of competition with other elements which have the same subscript  $i$  or  $j$ , and the parameter  $\alpha_0$  controls the strength of the competition. The third term suppresses solutions with low performance. This system is derived as a gradient system of a potential function  $V$ :

$$V = V_0 + V_1, \tag{6}$$

$$V_0 = \frac{1}{4} \sum_{i,j} (1 - u_{ij}^2)^2 + \frac{\alpha_0}{8} \sum_{i,j} \left[ \sum_{i' \neq i} u_{i'j}^2 + \sum_{j' \neq j} u_{ij'}^2 \right] u_{ij}^2, \tag{7}$$

$$V_1 = \frac{1}{4} \alpha_1 L(u_{ij}^2). \tag{8}$$

Let  $\bar{u}_{ij}$  ( $i, j = 1, \dots, N$ ) denote an equilibrium solution of the dynamical system (5a) and (5b), which is given by the following equations:

$$\bar{f}_{ij} = f_{ij}(\bar{u}_{i'j'}, \alpha_0, \alpha_1) = 0, \quad (i, j) \in \Gamma, \quad \bar{u}_{ij} = 0, \quad (i, j) \notin \Gamma, \tag{9}$$

where the set  $\Gamma$  of subscripts  $(i, j)$  ( $i, j = 1, \dots, N$ ) is defined as follows:

$$\Gamma = \{(i, j) | \bar{u}_{ij} \neq 0, i, j = 1, \dots, N\}. \tag{10}$$

Since  $f_{ij}$  is linear with respect to  $u_{ij}^2$ , the equilibrium solution  $\bar{u}_{ij}$  is obtained by solving the following linear algebraic equation:

$$C^\Gamma \mathbf{z}^\Gamma = \mathbf{b}^\Gamma, \tag{11}$$

where

$$\mathbf{z}^\Gamma = [\mathbf{x}^{\Gamma T} \mathbf{y}^{\Gamma T}]^T, \tag{12}$$

$$\mathbf{x}^\Gamma = [\dots \bar{u}_{ij}^2 \dots]^T, \quad (i, j) \in \Gamma, \quad \mathbf{y}^\Gamma = [\dots \bar{u}_{ij}^2 \dots]^T, \quad (i, j) \notin \Gamma, \tag{13}$$

$$\mathbf{b}^\Gamma = [\overbrace{1 \dots 1}^{n(\Gamma)} \overbrace{0 \dots 0}^{N^2 - n(\Gamma)}]^T, \tag{14}$$

$$C^\Gamma = \begin{bmatrix} C_x^\Gamma & 0 \\ 0 & I_{N^2 - n(\Gamma)} \end{bmatrix}, \tag{15}$$

and  $C_x^\Gamma$  is an  $n(\Gamma) \times n(\Gamma)$  matrix where  $n(\Gamma)$  indicates the number of elements of the set  $\Gamma$ . The matrix  $C_x^\Gamma$  is given in Appendix A.1. If the matrix  $C_x^\Gamma$  is singular, the equilibrium solution corresponding to the set  $\Gamma$  is not uniquely given. But for the general QAP in which the matrices  $A$  and  $B$  have no specific structure, it is considered that such a situation does not occur. So it is assumed in the following that the matrix  $C_x^\Gamma$  is nonsingular.

Equilibrium solutions of the dynamical system (5a) and (5b) are classified as follows:

$$\begin{aligned} \text{uniform solution : } & \Gamma = \Gamma^0, \\ \text{transition solution : } & \Gamma = \Gamma^t \neq \Gamma^0, \Gamma^p \quad \forall p \in \Pi_N, \\ \text{feasible solution : } & \Gamma = \Gamma^p, \quad p \in \Pi_N, \end{aligned} \quad (16)$$

where

$$\Gamma^0 = \{(i, j) | i, j = 1, \dots, N\}, \quad (17)$$

$$\Gamma^p = \{(i, j) | i = p(j); j = 1, \dots, N\}, \quad p \in \Pi_N. \quad (18)$$

The uniform solution is the equilibrium solution in which all of the elements have nonzero values. On the other hand, each of the feasible solutions corresponds to a permutation matrix and thus corresponds to an approximate solution of the QAP.

By linearizing the dynamical system (5a) and (5b) with respect to  $\delta u_{ij} = u_{ij} - \bar{u}_{ij}$  near the equilibrium solution corresponding to  $\Gamma$ , the following equation is obtained:

$$\delta \dot{\mathbf{u}}^\Gamma = D^\Gamma \delta \mathbf{u}^\Gamma, \quad (19)$$

where

$$\delta \mathbf{u}^\Gamma = [\delta \mathbf{u}_x^{\Gamma^T} \delta \mathbf{u}_y^{\Gamma^T}]^T, \quad (20)$$

$$\delta \mathbf{u}_x^\Gamma = [\dots \delta u_{ij} \dots]^T, \quad (i, j) \in \Gamma, \quad \delta \mathbf{u}_y^\Gamma = [\dots \delta u_{ij} \dots]^T, \quad (i, j) \notin \Gamma, \quad (21)$$

$$D^\Gamma = \begin{bmatrix} D_x^\Gamma & 0 \\ 0 & D_y^\Gamma \end{bmatrix}, \quad (22)$$

$$D_x^\Gamma = -2P^\Gamma C_x^\Gamma P^\Gamma, \quad D_y^\Gamma = \text{diag}(\bar{f}_{ij}), \quad (i, j) \notin \Gamma, \quad (23)$$

$$P^\Gamma = \text{diag}(|\bar{u}_{ij}|), \quad (i, j) \in \Gamma. \quad (24)$$

Since the matrix  $D^\Gamma$  is symmetric, stability of the equilibrium solution is verified by the following condition:

$$D^\Gamma < 0. \quad (25)$$

Stability conditions of each equilibrium solutions are summarized as follows: the sufficient condition for the uniform solution to be stable is given as follows:

$$0 < \alpha_0 < 1 - \frac{\alpha_1}{2} \max_{i,j} \sum_{i',j'} (a_{ij'} b_{i'i} + a_{j'j} b_{i'i}). \quad (26)$$

On the other hand, all equilibrium solutions except for the uniform solution are unstable if

$$0 < \alpha_0 < \frac{1}{N-1} \left\{ 1 - \frac{\alpha_1}{2} \max_{i,j} \sum_{i',j'} (a_{ij'} b_{i'i} + a_{j'j} b_{i'i}) \right\}. \quad (27)$$

Therefore, in the region where parameters  $\alpha_0, \alpha_1$  are sufficiently small, only the uniform solution is stable. The sufficient condition for all feasible solutions to be stable is given as follows:

$$\alpha_0 > \frac{1}{1 - \alpha_1(N - 1)}. \tag{28}$$

On the other hand, all equilibrium solutions except for the feasible solutions are unstable if

$$\alpha_0 > 2, \quad \alpha_1 < \frac{2}{\max_{i,j} \sum_{i',j'} (a_{jj'} b_{ii'} + a_{j'j} b_{i'i})}. \tag{29}$$

Therefore, only the feasible solutions are stable when  $\alpha_1$  is small and  $\alpha_0$  is large. Moreover, the stability condition for a feasible solution corresponding to a permutation  $p \in \Pi_N$  is approximately given as

$$\alpha_0 > 1 + \frac{\alpha_1}{N - 1} (L(p) - \bar{L}(p)), \tag{30}$$

$$L(p) = \sum_{j,j'} a_{jj'} b_{p(j)p(j')}, \tag{31}$$

$$\bar{L}(p) = \frac{1}{2N} \sum_{i,j,j'} (a_{jj'} b_{ip(j')} + a_{j'j} b_{p(j')i}), \tag{32}$$

where  $L(p)$  is the value of the performance index corresponding to the feasible solution and  $\bar{L}(p)$  corresponds to the mean value of the performance index in a neighborhood of the feasible solution. It has been clarified numerically that the mean value  $\bar{L}(p)$  is almost constant for any feasible solution. Then, the condition (30) is rewritten as

$$\alpha_0 > 1 + \frac{\alpha_1}{N - 1} (L(p) - \bar{L}), \quad \bar{L} : \text{constant}. \tag{33}$$

The condition (33) indicates that the feasible solutions become stable approximately according to the value of the performance index, and it has been clarified numerically that the condition (33) is a fairly good approximation.

#### 4. Bifurcation characteristics of the proposed model

In this section, we analyze the bifurcation structure of the equilibrium solutions of the dynamical system (5a) and (5b) with the parameter  $\alpha_0$  as the control parameter.

First, we consider the local bifurcation structure of the dynamical system (5a) and (5b). Choose a set  $\Gamma$ , and let  $\bar{u}_{ij} (i, j = 1, \dots, N)$  be the corresponding equilibrium solution. The existence of the equilibrium solution is verified by the condition that Eq. (11) has a non-negative solution. If the equilibrium solution exists, stability of the solution is verified by Eq. (25), i.e. by the sign of the eigenvalues of the matrix  $D^\Gamma$ . Here, we assume that at some point  $\alpha_0 = \bar{\alpha}_0$ , only one element  $\bar{u}_{i_1 j_1}$  of the solution  $\bar{u}_{ij}$  satisfies both of the following equations:

$$\bar{f}_{i_1 j_1} = 0 \quad \text{and} \quad \bar{u}_{i_1 j_1} = 0. \tag{34}$$

In this case, the matrix  $D^\Gamma$  has a simple zero eigenvalue. This assumption may be valid unless the matrices  $A, B$  have some specific structure. The linearized system (19) is rewritten as follows:

$$\begin{bmatrix} \delta \dot{\mathbf{u}}^\Gamma \\ \delta \dot{u}_{i_1 j_1} \end{bmatrix} = \begin{bmatrix} \hat{D}^\Gamma & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \delta \mathbf{u}^\Gamma \\ \delta u_{i_1 j_1} \end{bmatrix}, \tag{35}$$

where the  $(N^2 - 1)$ -dimensional vector  $\delta\hat{\mathbf{u}}^\Gamma$  is given by removing the element  $\delta u_{i_1 j_1}$  from the  $N^2$ -dimensional vector  $\delta\mathbf{u}^\Gamma$  and  $\hat{D}^\Gamma$  is an  $(N^2 - 1) \times (N^2 - 1)$  nonsingular matrix derived by removing the row and the column corresponding to  $(i_1, j_1)$  from  $D^\Gamma$ . There exists a one-dimensional center manifold  $W^c$  tangent to the one-dimensional center subspace spanned by the eigenvector corresponding to the zero eigenvalue [13]. In this case, the center subspace is the  $u_{i_1 j_1}$ -axis and the center manifold  $W^c$  can be represented as a local graph:

$$W^c = \{(\delta\hat{\mathbf{u}}^\Gamma, \delta u_{i_1 j_1}, \delta\alpha_0) | \delta\hat{\mathbf{u}}^\Gamma = \mathbf{g}(\delta u_{i_1 j_1}, \delta\alpha_0)\}, \tag{36}$$

where  $\delta\alpha_0 = \alpha_0 - \bar{\alpha}_0$  and  $\mathbf{g}(\delta u_{i_1 j_1}, \delta\alpha_0)$  is an  $(N^2 - 1)$ -dimensional vector-valued function of  $\delta u_{i_1 j_1}$  and  $\delta\alpha_0$  defined on some neighborhood of the bifurcation point  $(\bar{u}_{ij}, \bar{\alpha}_0)$ . The graph  $\mathbf{g}(\delta u_{i_1 j_1}, \delta\alpha_0)$  is expanded in a Taylor series at the bifurcation point as follows:

$$\mathbf{g} = \delta u_{i_1 j_1}^2 \mathbf{w}_u^\Gamma + \delta\alpha_0 \mathbf{w}_\alpha^\Gamma + O(|\delta u_{i_1 j_1}|^3). \tag{37}$$

The coefficient vectors  $\mathbf{w}_u^\Gamma, \mathbf{w}_\alpha^\Gamma$  are determined by the following equations:

$$\hat{D}^\Gamma \mathbf{w}_u^\Gamma = \mathbf{h}_u^\Gamma, \quad \hat{D}^\Gamma \mathbf{w}_\alpha^\Gamma = \mathbf{h}_\alpha^\Gamma, \tag{38}$$

where the vectors  $\mathbf{h}_u^\Gamma, \mathbf{h}_\alpha^\Gamma$  are given in Appendix A.2. The one-dimensional reduced dynamical system on the center manifold  $W^c$ , which determines the local behavior of the dynamical system (5a) and (5b) near the bifurcation point, is given by

$$\delta\dot{u}_{i_1 j_1} = \mu_1 \left( \delta\alpha_0 + \frac{\mu_2}{\mu_1} \delta u_{i_1 j_1}^2 \right) \delta u_{i_1 j_1} + O(|\delta u_{i_1 j_1}|^4), \tag{39}$$

where constants  $\mu_1, \mu_2$  are given in Appendix A.3. The normal form (39) shows that the bifurcation is the pitchfork bifurcation. There are two types of pitchfork bifurcations, i.e. the supercritical (when  $\mu_2 < 0$ ) and the subcritical (when  $\mu_2 > 0$ ) pitchfork bifurcations. In the pitchfork bifurcations, there are two branches of equilibrium solutions with nonzero values: one has positive values and another has negative values. In this case, since the performance index is the function of  $u_{ij}^2$ , the performance of the solution is not affected by this uncertainty. By analyzing the local bifurcation structure of the system, it is revealed that under the assumption (34), only the pitchfork bifurcations occur in the system.

Next, we consider the global bifurcation structure of the system. Fig. 1 is the schematic global bifurcation diagram. The uniform solution exists in the region where  $\alpha_0$  is small. When the value of  $\alpha_0$  is increased, the uniform solution becomes unstable and a transition solution becomes stable through a supercritical pitchfork bifurcation (labeled as “a” in Fig. 1). Then, by increasing the value of  $\alpha_0$ , other transition solutions appear through subcritical pitchfork bifurcations. By increasing the value of  $\alpha_0$  furthermore, feasible solutions become stable through supercritical pitchfork bifurcations or appear through subcritical pitchfork bifurcations (labeled as “b” in Fig. 1). Among these branches, there is a branch with which the uniform solution connects through supercritical and subcritical pitchfork bifurcations

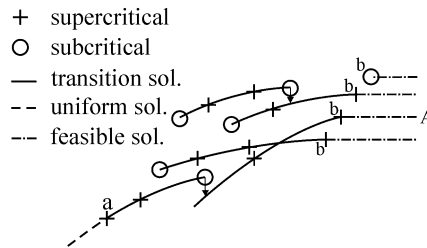


Fig. 1. Schematic global bifurcation diagram.

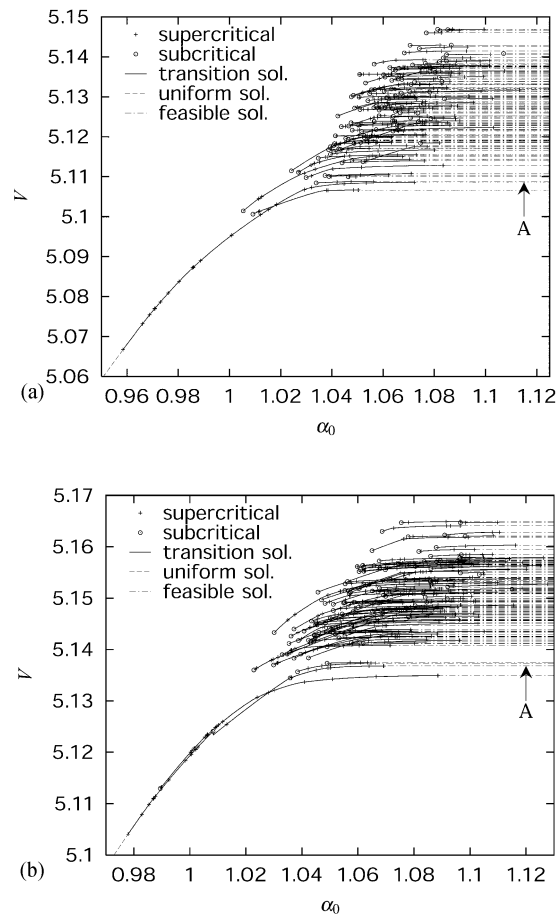


Fig. 2. Global bifurcation diagrams.

when the value of  $\alpha_0$  is increased (the branch A in Fig. 1). Figs. 2(a) and (b) show two examples of the global bifurcation diagrams, where  $N = 5$  and matrices  $A, B$  are randomly generated. In the figures, three types of branches are drawn: one is a branch starting from the uniform solution and connecting with a feasible solution. Another is a branch starting from a transition solution and connecting with the optimal solution. The others are branches starting from transition solutions and connecting with feasible solutions. In the case of Fig. 2(a), the uniform solution connects with a feasible solution only through supercritical pitchfork bifurcations. The feasible solution connected with the uniform solution is the second best solution. On the other hand, in the case of Fig. 2(b), the uniform solution connects with a feasible solution through one supercritical and two subcritical pitchfork bifurcations. The feasible solution connected with the uniform solution is the second best solution. From the analysis of the global bifurcation structure of the system, it is revealed that there is a feasible solution with which the uniform solution connects. From numerical experiments, in many cases, the feasible solution is a good approximate solution of the optimization problem.

## 5. Deterministic annealing algorithm

Based on the analysis of bifurcation characteristics, we propose the following deterministic annealing algorithm to obtain a good approximate solution for the QAP. The purpose of the proposed algorithm is to trace the branch

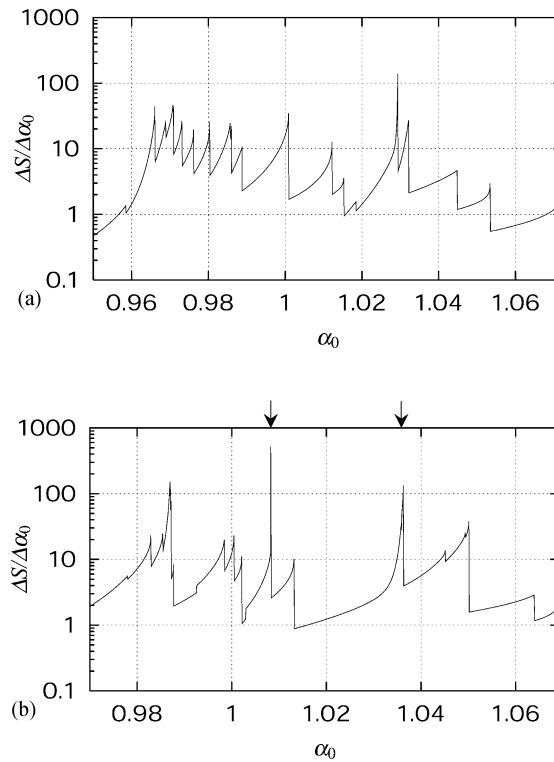


Fig. 3. Change of the parameter  $S$  with respect to the parameter  $\alpha_0$ . Arrows in (b) indicate the points where the subcritical pitchfork bifurcations occur.

starting from the uniform solution and connecting with a feasible solution accurately and efficiently. The algorithm is carried out as follows:

- Step 1: Set  $\alpha_0$  sufficiently small and compute Eqs. (5a) and (5b) to obtain the uniform solution.
- Step 2: Slightly increase  $\alpha_0$ .
- Step 3: Compute Eqs. (5a) and (5b) with the solution of the previous iteration as the initial value to obtain the equilibrium solution.
- Step 4: Go to Step 2 until the feasible solution is obtained.

To accurately trace the branch connecting the uniform solution with a feasible solution, the increments of the parameter  $\alpha_0$  must be sufficiently small. However, too small increments of  $\alpha_0$  increase the computation time. Therefore, to control the increment of the parameter  $\alpha_0$ , we introduce the following parameter  $S$ :

$$S = -\frac{1}{N \log N} \sum_{i,j} p_{ij} \log p_{ij}, \quad p_{ij} = \frac{u_{ij}^2}{\sum_{j'} u_{ij'}^2}, \quad (40)$$

where  $p_{ij}$  is normalized so that the sum over  $j$  is equal to unity. The parameter  $S$  takes the maximum value of 1 for the uniform solution and the minimum value of 0 for feasible solutions. Figs. 3(a) and (b) show the change of the parameter  $S$  for the branch connecting the uniform solution with a feasible solution when the value of  $\alpha_0$  is increased, where cases (a) and (b) in Fig. 3 correspond to cases (a) and (b) in Fig. 2, respectively. These



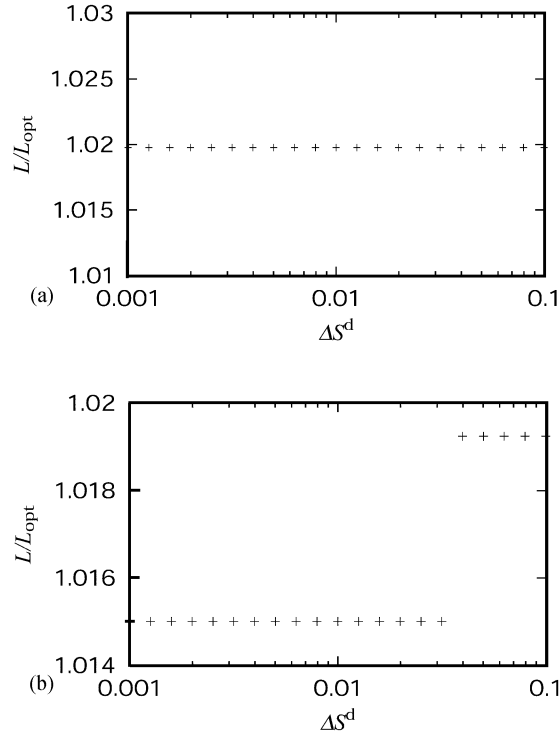


Fig. 4. Values of the performance index obtained by the proposed algorithm.

figures show that the parameter  $S$  changes sharply at the point where a bifurcation occurs. Especially, the amount of the change is largest at the point where a subcritical pitchfork bifurcation occurs. Using the parameter  $S$ , the increment of the parameter  $\alpha_0$  in Step 2 is controlled so that the amount of the change of the parameter  $S$  is kept constant:

$$\Delta\alpha_0 = \frac{\Delta S^d}{\Delta S} \Delta\alpha_0^{old}, \quad (41)$$

$$\Delta\alpha_0 = \alpha_0 - \alpha_0^{old}, \quad \Delta S = |S - S^{old}|, \quad (42)$$

where  $\Delta S^d$  is the desired change of the parameter  $S$  and  $\alpha_0^{old}$ ,  $S^{old}$  represent the previous values of each parameter. By using the parameter  $S$ , the value of the parameter  $\alpha_0$  is increased more slowly at points where the subcritical pitchfork bifurcations occur. Results of the proposed deterministic annealing algorithm for the above examples are shown in Figs. 4(a) and (b). In each figure, the values of the performance index  $L$  over 100 trials of the algorithm are plotted against various values of  $\Delta S^d$  where the initial values are generated randomly.  $L_{opt}$  is the optimal value of  $L$ . In case (a), where no subcritical pitchfork bifurcation occurs during the annealing process, the feasible solution with which the uniform solution connects is obtained for all values of  $\Delta S^d (\leq 1)$  and in all trials. On the other hand, in case (b) where subcritical pitchfork bifurcations occur, a feasible solution other than the above solution is obtained when  $\Delta S^d$  is large. However, by setting  $\Delta S^d$  sufficiently small, the feasible solution with which the uniform solution connects is always obtained.

Table 1  
Values of the performance index obtained by our method

Name	$N$	$L_{opt}$ (algorithm)	$L$	Difference (%)
Sko56	56	34458 (Ro-TS)	34502	0.13
Sko100a	100	152002 (GEN)	152502	0.33
Tai50a	50	4941410 (GEN)	5051386	2.2
Tai50b	50	458821517 (Ro-TS)	459975270	0.25
Tai80a	80	13557864 (Ro-TS)	13733524	1.3
Tai80b	80	818415043 (Ro-TS)	821025553	0.32
Tai100b	100	1185996137 (Ro-TS)	1193847431	0.66
Tho150	150	8133484 (SIMJ)	8158137	0.30
Wil50	50	48816 (SIM)	48892	0.16
Wil100	100	273038 (GEN)	273294	0.094

## 6. Experiments

The proposed deterministic annealing algorithm is applied to problem instances in the QAPLIB [14]. Some of the results are shown in Table 1. The third column ( $L_{opt}$ ) of the table is the value of the performance index of the best known solution given in QAPLIB, and in parentheses we show the name of the algorithm which obtained the solution, i.e. robust Tabu search (Ro-TS), genetic hybrids (GEN), simulated annealing (SIM) and simulated jumping (SIMJ). The fourth column ( $L$ ) is the solution obtained by the proposed method, and the fifth column is the relative difference (%),  $100(L - L_{opt})/L_{opt}$ . Table 1 shows that the relative difference is less than 1% for most problem instances and therefore the performance of the proposed method is comparable to other heuristic methods. Table 2 shows the comparison with other methods using dynamical systems, i.e. Potts mean field theory annealing (PMA) [5,6], doubly constrained network annealing (DCA) [6] and  $\lambda$ -doubly constrained network ( $\lambda$ -DCN) [8]. The values for these methods are taken from [6,8]. In the table, “–” means that the method could not obtain good solutions in a reasonable time, and there are no data for the problem instance “Tai50a” by  $\lambda$ -DCN in the reference. The best solutions among these methods are in italic. Table 2 shows that the performance of the proposed method is comparable to other methods using dynamical systems.

The CPU time to obtain one feasible solution on a DEC Alpha Station 500/333 is about 2 min for  $N = 20$ , 30 min for  $N = 40$  and 8 h for  $N = 80$ .

Lastly, the difficulties of tuning the values of parameters should be mentioned. In this algorithm, the important parameters to be set are  $\alpha_1$  and  $\Delta S^d$ . The value of the parameter  $\alpha_1$  is determined so that the annealing starts from the uniform solution and is set based on the short preliminary computation. The parameter  $\alpha_1$  is robust against the performance of the solution obtained. The value of the parameter  $\Delta S^d$  is determined so that the feasible solution connected with the uniform solution is obtained. From the experiments, the parameter  $\Delta S^d$  is robust against the size of the problem and the recommended value is  $\Delta S^d = 0.01$ . Therefore, it is not so difficult and troublesome to set parameters in the proposed algorithm.

Table 2  
Comparison with other methods using dynamical systems

Name	PMA	DCA	$\lambda$ -DCN	Our method
Tai50a	4.3	2.7	*	2.2
Tai80a	–	1.2	<i>–0.060</i>	1.3
Wil100	–	0.27	0.46	<i>0.094</i>
Tho150	–	0.33	<i>0.24</i>	0.30

### 7. Conclusion

We have proposed a deterministic annealing algorithm for a combinatorial optimization problem based on successive bifurcation characteristics of a replicator equation. First, the bifurcation structure of the proposed dynamical system was analyzed in detail. It was shown that only pitchfork bifurcations occur in this model. It was also clarified that there is a feasible solution uniquely connected with the uniform solution, and the solution is a good approximate solution. Then, we proposed a deterministic annealing algorithm which starts from the uniform solution and reaches the feasible solution connecting with the uniform solution. In the algorithm, the feasible solution obtained is unique and a good approximate solution because of the bifurcation characteristics of the proposed model. The annealing schedule is determined based on the bifurcation characteristics and there is no difficulty in setting parameters in the algorithm. Results of numerous tests showed the high performance of this algorithm.

### Appendix A

#### A.1. Definition of the matrix $C_x^\Gamma$

The matrix  $C_x^\Gamma$  in Eq. (15) is given by removing columns and rows which correspond to  $(i, j) \notin \Gamma$  from the following  $N^2 \times N^2$  matrix  $C$ :

$$C = C_0 + C_1, \tag{A.1}$$

$$C_0 = \begin{bmatrix} C_0^{(1)} & C_0^{(2)} & \dots & C_0^{(2)} \\ C_0^{(2)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & C_0^{(2)} \\ C_0^{(2)} & \dots & C_0^{(2)} & C_0^{(1)} \end{bmatrix}, \tag{A.2}$$

$$C_0^{(1)} = \begin{bmatrix} 1 & \frac{1}{2}\alpha_0 & \dots & \frac{1}{2}\alpha_0 \\ \frac{1}{2}\alpha_0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{1}{2}\alpha_0 \\ \frac{1}{2}\alpha_0 & \dots & \frac{1}{2}\alpha_0 & 1 \end{bmatrix}, \quad C_0^{(2)} = \frac{1}{2}\alpha_0 I_N, \tag{A.3}$$

$$C_1 = \begin{bmatrix} C_1^{(11)} & \dots & C_1^{(1N)} \\ \vdots & \ddots & \vdots \\ C_1^{(N1)} & \dots & C_1^{(NN)} \end{bmatrix}, \quad (C_1^{(ij)})_{i'j'} = \frac{1}{2}\alpha_1 (a_{jj'} b_{i'i} + a_{j'i} b_{i'j}). \tag{A.4}$$

#### A.2. Definitions of vectors $\mathbf{h}_u^\Gamma$ and $\mathbf{h}_\alpha^\Gamma$

$\mathbf{h}_u^\Gamma, \mathbf{h}_\alpha^\Gamma$  in Eq. (38) are  $(N^2 - 1)$ -dimensional vectors given as follows:

$$\mathbf{h}_u^\Gamma = \left[ \overbrace{\mathbf{h}_{ux}^{\Gamma^T}}^{n(\Gamma)} \quad \overbrace{\mathbf{h}_{uy}^{\Gamma^T}}^{N^2-n(\Gamma)-1} \right]^T, \tag{A.5}$$

$$\mathbf{h}_\alpha^\Gamma = \left[ \overbrace{\mathbf{h}_{\alpha x}^{\Gamma T}}^{n(\Gamma)} \quad \overbrace{\mathbf{h}_{\alpha y}^{\Gamma T}}^{N^2-n(\Gamma)-1} \right]^T, \quad (\text{A.6})$$

$$\mathbf{h}_{ux}^\Gamma = [\cdots h_{u,ij}^\Gamma \cdots]^T, \quad (i, j) \in \Gamma, \quad \mathbf{h}_{uy}^\Gamma = [0 \cdots 0]^T, \quad (\text{A.7})$$

$$\mathbf{h}_{\alpha x}^\Gamma = [\cdots h_{\alpha,ij}^\Gamma \cdots]^T, \quad (i, j) \in \Gamma, \quad \mathbf{h}_{\alpha y}^\Gamma = [0 \cdots 0]^T, \quad (\text{A.8})$$

$$h_{u,ij}^\Gamma = -\frac{1}{2}\bar{\alpha}_0(\delta_{ii_1} + \delta_{jj_1})\bar{u}_{ij} - \frac{1}{2}\alpha_1(a_{j_1j'}b_{i_1i'} + a_{j_1j}b_{i_1i})\bar{u}_{ij}, \quad (i, j) \in \Gamma, \quad (\text{A.9})$$

$$h_{\alpha,ij}^\Gamma = -\frac{1}{2} \left[ \sum_{\substack{i' \neq i \\ (i', j) \in \Gamma}} \bar{u}_{i'j}^2 + \sum_{\substack{j' \neq j \\ (i, j') \in \Gamma}} \bar{u}_{ij'}^2 \right] \bar{u}_{ij}, \quad (i, j) \in \Gamma, \quad (\text{A.10})$$

where  $\delta_{ii_1}, \delta_{jj_1}$  are the Kronecker's delta.

### A.3. Definitions of the constants $\mu_1$ and $\mu_2$

The constants  $\mu_1, \mu_2$  in Eq. (39) are given as follows:

$$\begin{aligned} \mu_1 = & -\bar{\alpha}_0 \left[ \sum_{\substack{i' \neq i_1 \\ (i', j_1) \in \Gamma}} \bar{u}_{i'j_1} w_{\alpha, i'j_1} + \sum_{\substack{j' \neq j_1 \\ (i_1, j') \in \Gamma}} \bar{u}_{i_1j'} w_{\alpha, i_1j'} \right] - \alpha_1 \sum_{\substack{i', j' \\ (i', j') \in \Gamma}} (a_{j_1j'} b_{i_1i'} + a_{j'j_1} b_{i'i_1}) \bar{u}_{i'j'} w_{\alpha, i'j'} \\ & - \frac{1}{2} \left[ \sum_{\substack{i' \neq i_1 \\ (i', j_1) \in \Gamma}} \bar{u}_{i'j_1}^2 + \sum_{\substack{j' \neq j_1 \\ (i_1, j') \in \Gamma}} \bar{u}_{i_1j'}^2 \right], \end{aligned} \quad (\text{A.11})$$

$$\begin{aligned} \mu_2 = & -\bar{\alpha}_0 \left[ \sum_{\substack{i' \neq i_1 \\ (i', j_1) \in \Gamma}} \bar{u}_{i'j_1} w_{u, i'j_1} + \sum_{\substack{j' \neq j_1 \\ (i_1, j') \in \Gamma}} \bar{u}_{i_1j'} w_{u, i_1j'} \right] \\ & - \alpha_1 \sum_{\substack{i', j' \\ (i', j') \in \Gamma}} (a_{j_1j'} b_{i_1i'} + a_{j'j_1} b_{i'i_1}) \bar{u}_{i'j'} w_{u, i'j'} - (1 + \alpha_1 a_{j_1j_1} b_{i_1i_1}). \end{aligned} \quad (\text{A.12})$$

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