AN ANT-BASED SELF-ORGANIZING FEATURE MAPS ALGORITHM

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Abstract – *Kohonen's Self-Organizing feature Maps (SOMs) have been well-known as an excellent tool for data mining during the exploratory phase. Regarding to the mapping in the conventional SOM algorithm for an input data, the best matching unit is simply determined on the basis of the Euclidian distances between the input data vector and the map unit vectors. In this research, we propose a novel algorithm, named Ant-Based of Self-Organizing feature Maps algorithm (ABSOM), which combines the ant colony system of swarm intelligence and the Kohonen's SOM for data clustering. The ABSOM utilizes the pheromone mechanism of ant colony system to memorize the history of the best matching units selected. Besides, the ABSOM adopts the state transition rules of exploitation and exploration to determine the best matching unit on the map topology, instead of the shortest Euclidean distance. After the comparisons between the ABSOM and the Kohonen's SOM on four data sets: the iris ,wine , pen-based, and optical data set, we confirm the proposed algorithm is prominent in overcoming the local minimum problem and provide the superior characteristic in map resolution.*

Key words –Self-Organizing Feature Map, Ant Colony System, Data Mining, Clustering Analysis.

1 Introduction

Clustering analysis is one of the most important research issues in data mining domain and also very useful for many applications, such as marketing, industrial engineering and image processing, biology, medicine. At present, there are many new clustering algorithms that were created by combining the traditional statistical methods with Artificial Intelligence (AI), e.g. neural networks, genetic algorithms, fuzzy sets theory, and ant colony systems. In the neural network aspect, the Kohonen's SOMs project the input data set in the input data space to a lower dimensional regular grid that can be used effectively in the data visualization and the property exploration phase of data mining. Hence, the SOM is generally acknowledged an excellent tool in data mining. Furthermore, another new research field of artificial intelligence is so-called swarm intelligence, which is a field studing "the emergent collective intelligence of groups of simple agents" [1]. In their researches, the group of insects can only do simple tasks. The blind-liked insects such as the ants and the bees, however, could communicate with each other just like the mankind by means of the chemical substance called pheromone. Based on the above idea, Dorigo et al. [8] proposed an algorithm named Ant System (AS), a new approach of stochastically combinatorial optimization. And then in 1997, the consequent study of the AS called the Ant

Colony System (ACS) was introduced. The main difference between these two systems is that ant colony can effectively avoid the local minimum problem and find a better and near optimal solution. Taking advantage of the superior features of ACS, the purpose of this research, therefore, is to develop an advanced ant-based SOM algorithm, which integrates the ACS and SOM .

The structure of this paper is organized into four sections. In Section 1, the brief description about the background of this research is first introduced. In Section2, the SOM, AS and ACS algorithms are comprehensively reviewed. In Section 3, the proposed ant-based SOM algorithm is described in detail. In Section 4, the practical study of the proposed methodology using four previous data sets provided in a clustering database will be demonstrated and compared with SOM. Finally, the conclusions of this research are presented in Section 5.

2 Literature Review

In this section, the AS, ACS and SOM are reviewed.

2.1 AS and ACS

As the initialization of other AI techniques, the foraging behavior of the real ants inspires to create the AS algorithm. There are three main facts forming the natural ant behaviors: (a) the ants communicate with each other through pheromone, (b) the shorter path is, the higher rate of pheromone growth is, and (c) the more pheromone left behind on the path , the more preferred the ant choose it [7]. In the process of searching food, the ants will lay the chemical substances called 'pheromones' on the paths as they go through. Consequently, the ants cooperate using the indirect form of communication mediated by pheromone trails. After building an edge, the ants choose the next node (or city) to move using a probability-oriented function which is determined by the length of the tour. In other words, the shorter the tour is, the more pheromone lying on it. Ant system has been employed to some combinatorial problems such as travel salesman problem(TSP) [5,6,8,20], as well as quadratic assignment problem [17,19]., and proved that it's more promising than other heuristics like GA, Evolutionary Programming (EP), Simulated Annealing (SA), and SOMs [7].

Although the AS was useful for discovering good or near optimal solutions for the TSPs, the time required to find such results made it unfeasible for large problems [7]. Hence in 1997, the further researches, built on the basis of the previous AS for improving the efficiency of solving the TSP problems, were continued and the advanced system was named the Ant Colony System (ACS). The main differences between the AS and ACS are the global pheromone updating rule, the state transition rule, and the local pheromone updating rule. In the progenitor of the ACS, the global updating rule was utilized on all edges once all the ants had completed their tours. But in the ACS, this rule is only used for the best ant tour. Secondly, before performing the global updating rule, the ACS adds the local updating rule while the ant constructs a solution. When the ant moves from a city to the next, the pheromone lying on the edge will be updated first. In addition, the modifications of the state transition rule include the exploration of new edges and the exploitation of priori ants accumulated information. Being added the exploration strategy, shown as Fig. 1, the ACS can avoid the local minimum and find the relatively better solutions than the AS. And this part is just our inspiration to combine with another promising algorithm, i.e. SOM, for clustering domain.

In the ACS algorithm, the state transition rule is employed as an ant k moves from node r to the next city s, where $J_k(r)$ is the set of the cities still unvisited on node r, and β is the relative importance parameter of pheromone $\tau(t)_{(r,u)}$ versus distance $\eta(r,u)$ from city r to city u, where $u \in J_k(r)$. After the next city s having been chosen using the transition rule, the new pheromone

$\tau(t+1)_{(r,u)}$ between the cities r and u are updated in terms of the last pheromone $\tau(t)_{(r,u)}$, the amount of updating pheromone $\Delta\tau(t+1)_{(r,u)}$ and the learning coefficient of local updating ρ. In the formula of $\Delta\tau(t+1)_{(r,u)}$, the term of Q represents the total pheromone capacity of an ant, which is usually set to be a constant. As all the ants have visited all the cities, only the best tour s will be executed the global updating. In other words, the pheromone of other tours will be decreased by the ratio $(1-\alpha)$.

The development of Ant Colony Optimization (ACO) meta-heuristic [6], which represents a particular class of ant algorithms, has become a new research issue within the recent years. As pointed by the literatures, the ant algorithms have been one of the most successful algorithms of swarm intelligent system [2], and have been employed to many fields, such as the classical TSP, scheduling, vehicle routing and quadratic assignment problems. With the superior features pointed above, the ant algorithms have been employed for data mining by more and more researchers. For instance, Yuqing et al. [27] proposed a novel K-Means algorithm based on density and ant algorithm, which apply ant-based clustering to create an initial cluster and then K-Means is followed. This two-level resolved the problem of local minimum by the multi-point searching capability of ant algorithm and enable to handle the sensitivity problem of the initial parameters settings in K-Means. Besides, Chelokar et al. [3] and Yang et al. [26] recasted the ACO algorithm to meet the requirement for data clustering. Also, Tsai et al.[4] adopted the ACO to decide different probability of the next city to be chosen, utilize the simulated annealing concept that decreases the number of visit cities, and uses tournament selection strategy to improve the probability function in ACO. Employed for data mining, the ant algorithms can not long be used for clustering analysis but data classification. For example, Parpinelli et al. [18] utilized the ACO in the context of rule discovery to perform a flexible and robust search of the combination of terms involving values of the predictor attributes. Wu and Shi [25] employed the Deneubourg's model for clustering to develop the Clustering based on Swarm Intelligence (SCI) model through the combination of the swarm similarity, swarm similarity coefficient and probability conversion function.

Initialize parameters setting
While (stop criteria do not meet)
  Each ant is positioned on a starting node
While
  Apply the state transition rule for each ant to search for a feasible solution and update the pheromones using the local updating rule

$$s = \begin{cases} \arg\max\{[\tau(t)_{(r,u)}]\cdot[\eta(r,u)]^{\beta}\} & ,if\ q \le q_0 \quad \text{(exploitation)} \\ P_k = \dfrac{[\tau(t)_{(r,u)}]\cdot[\eta(r,u)]^{\beta}}{\sum_{u\in J_k(r)}[\tau(t)_{(r,u)}]\cdot[\eta(r,u)]^{\beta}} & ,otherwise\ \text{(exploration)} \end{cases},$$

$$\Delta\tau(t+1)_{(r,u)} = \begin{cases} \dfrac{Q}{\eta(r,u)}, & \text{if } u = s \\ 0, & \text{otherwise} \end{cases}$$

$$\tau(t+1)_{(r,u)} = (1-\rho)\tau(t)_{(r,u)} + \rho\cdot\Delta\tau(t+1)_{(r,u)}$$

End
  Update the pheromone of the best solution using the global updating rule

$$\tau(t+1)_{(r,s)} = (1-\alpha)\tau(t)_{(r,s)} + \alpha\cdot\Delta\tau(t+1)_{(r,s)}$$

End

Fig. 1 The main portion of the ACS algorithm (reorganized from Dorigo, 1997)

2.2 Self-Organizing Feature Map

SOM was first introduced by T. Kohonen in 1981 [10,12-15]. It is an unsupervised neural network method which has the properties of both vector quantization and vector projection algorithms. It can be used for various applications such as pattern recognition, biological modeling, data compression, signal processing and data mining [13,23]. SOM is an orderly mapping technique which enables to map a high-dimensional data distribution in the input space onto a regular low-dimensional grid structure, usually one or two dimensional. The benefit of SOM is that it can create a set of prototype vectors which are the most suitable to represent the input data vectors. Generally speaking, it is capable of converting the complex, non-linear and high-dimensional data into simple, geometric and low-dimensional data which people can easily visualize. Therefore, SOM is especially suitable for data exploration in data mining [14,15].

As the modifications had been proposed, the SOM family owns a number of variants. The category of most SOM variants can be classified in terms of the following two factors: prototype vector and neighborhood relations [23]. Kangas et al. [9] utilized dynamic weighting of the input signals at each input cell which improves the ordering when very different input signals are used. Beside, the concept of Minimal Spanning Tree was also used in their approach to define the neighborhood in the learning algorithm. When compared with the hierarchical clustering methods, the SOM is additionally able to identify the tendency of classification errors when empirical data differentiate from the ideal conditions of the isolated clusters [16]. In Vesanto and Alhoniemi(2000) , a two-stage algorithm was proposed. The data input set was first clustered using the SOM at the first stage, and then the SOM is clustered to overcome the dilemma as result is similar to the original data after using the SOM. [22].

In this research, we propose an algorithm named Ant-Based Self-Organizing feature Maps (ABSOM) algorithm for data clustering. The ABSOM algorithm owns the original capability of SOM and two essential features from the ant algorithm: (a) the memorization of the historical winning output units by means of the pheromone mechanism of the ACO, (b) the appropriate state transition accoridng to the exploitation and exploration rules to determine the best matching output unit on the map topology, instead of using the shortest Euclidean distance.

3 Methodology

In this section, network structure, the mathematical terms and initial parameters of the proposed ABSOM are first of all defined and described in the following.

3.1 Terminological Definitions

(a) Topological network setting

Define the topological network $M = \{c_1, c_2 ... c_j ... c_m\}$, in which M consists of m = $m_1 \times m2$ map units where m_1 and m_2 represent respectively the number of units located on the two sides of the network. According to the probability distribution $P(\xi)$ where ξ stands for an input data, the n-dimensional weight vector $w_{c_j} \in R^n$ of every map unit c_j is initialized. Set the start time $t = 0$ and the initial neighborhood radius λ_0.

(b) Pheromone matrix setting

Construct a pheromone matrix $T = \{\tau_{c_1}, \tau_{c_2}, ..., \tau_{c_j}, ..., \tau_{c_m}\}$ and give each element of the matrix an initial pheromone $\tau_0 = 0$. Define q_0 to be the pheromone threshold of choosing the exploitation or exploration pheromone rule. The value of q_0 is ranged within [0, 1].

(c) Other parameters setting

N_{dlen}, $N_{trainlen}$, represent the number of total data samples and total training epochs, respectively. D_{c_j} is defined to be the set of data samples mapped on the map unit c_j.

3.2 The ABSOM Algorithm

The detailed steps of the proposed ABSOM algorithm, shown in Fig. 2, can be described as follows:

Step1 : Read in and normalize the training data set.

Step2 : Compute all the neighborhood radii that will be used during the training processes.

Step3 : Select a sample randomly and calculate the accumulative Euclidean distance δ_{ji} and pheromone T between the map units ϖ_j on the topological network and the input vector ξ_i.

$$\Delta\delta_{ji}(t) = \sum_{i=1}^{N_{batch}} \sum_{j}^{munits} \sum_{k}^{\dim} \left\| \xi_{ik} - \varpi_{jk}(t) \right\| \tag{1}$$

$$\tau_{c_j}(t+1) = \tau_{c_j}(t) + \Delta\delta_{c_j}(t) \tag{2}$$

Step4 : Conduct the updating processes for the weight vectors

(a) After the set of data samples mapped on the map units, find out the Best Match Unit (BMU) s for each data sample according to the following formula based on the exploitation and exploration updating rules of the ant-based algorithm:

$$s = \begin{cases} \arg\min \ \Delta\delta_{ji}(t), & \text{if } q \le q_0 \qquad \text{(exploitation)} \\ p_{c_j} = \dfrac{\tau_{c_j}(t+1)}{\sum_{c_j=c_1}^{c_j=c_N} \tau_{c_j}(t+1)}, & \text{otherwise} \qquad \text{(exploration)} \end{cases} \tag{3}$$

where q : a real number generated randomly from 0 to 1;

q_0 : the threshold to choose the exploitation updating rule when q is no greater than q_0;

p_{c_j} : the probability that the map unit c_j to be the BMU when the exploration rule is chosen.

To record the data samples that have mapped on the unit c_j, the accumulated data set can be expressed as

$$D_{c_j}(t+1) = \begin{cases} \{D_{c_j}(t), \xi_i\}, & \text{if } c_j = s \\ \{D_{c_j}(t)\}, & otherwise \end{cases} \tag{4}$$

(b) Calculate the distance between s and c_j

(c) Update the pheromone for each map unit

$$\tau_{c_j}(t+1) = \begin{cases} \beta\tau_{c_j}(t) + \alpha\Delta\tau_{c_j}(t+1), & \text{if } c_j = s \\ \beta T_{c_j}(t), & \text{otherwise} \end{cases} \tag{5}$$

where α: the accumulating rate of pheromone from the Euclidean distance; β: the decay rate of pheromone.

(d) Update the weight vector for each map unit

$$\Delta w_{c_j}(t) = lr(t)\cdot(\xi_i - w_s)\cdot h_{rs}(t) \tag{6}$$

where $lr(t)$ is the learning rate of connection weights at time t.

$$w_{c_j}(t+1) = w_{c_j}(t) + \Delta w_{c_j}(t) \tag{7}$$

Step5： Decrease the neighborhood radius and update the neighborhood coefficient

$$\lambda(t+1) = \varepsilon\lambda(t) \tag{8}$$

$$h_{rs} = f(r_{c_j}, \lambda(t)) = \exp(-r_{c_j} / \lambda(t)) \tag{9}$$

where $\lambda(t)$: the neighborhood radius at time t;

ε: the decreasing learning rate of neighborhood radius $\varepsilon \in (0,1)$;

r_{c_k}: the topological distance between the winner (or the BMU) and the unit c_j on the map topology.

Step6：Check the stopping criterion

4 Practical Study

To verify the performance of the proposed algorithm, four data sets had been applied and executed on a desktop PC with Pentium CPU. These data sets are Fisher's iris data (abbreviated by Iris), Forina's wine recognition data (abbreviated by Wine), optical recognition of handwritten digits (abbreviated by Optical) and pen-based recognition of handwritten digits (abbreviated by Pen-Based), which can be downloaded from the following website: [21].

The performance evaluation for the proposed SOM-based methodology is still a complicated issue. In order to compare the performances between the proposed ABSOM and the conventional Kohonen's SOM, this research adopts two typical properties: map resolution and topology preservation [11,12]. For these two properties, there are many ways to measure. For simplicity, this research chooses quantization error (QE), which is the average distance of all the input data vectors and their corresponding BMUs, and topographic error (TE), which is the proportion of all the data vectors for which first and second BMUs are not adjacent units.

In this section, what we desire to know is if the proposed ABSOM really performed better than the conventional SOM. As mentioned in Section 3.3, the performance of the ABSOM will be evaluated by comparing with that of the Kohonen's SOM, using the CIS SOM Toolbox 2.0 [24], according to the results from the four data sets. The proposed ABSOM is programmed in the Matlab 7.0 environment. The experiments for the four data sets are repetitively carried out ten times using these two algorithms. The best, worst and average results of the QE, TE indices after the ten repetitive experiments for each data set are shown in Table 1

Table 1 The results of QE, TE indices after ten repetitive experiments for the four data sets

Data Set	Iris		Wine		Pen-Based		Optical	
Algorithm	SOM	ABSOM	SOM	ABSOM	SOM	ABSOM	SOM	ABSOM
M.Q.E. (Best)	0.0839	**0.0810**	0.5021	**0.4971**	0.0209	**0.0056**	0.0744	**0.0419**
M.Q.E. (Worst)	0.0874	**0.0873**	0.5177	**0.5102**	0.0787	**0.0618**	0.1302	**0.1255**
M.Q.E (Avg.)	0.0857	**0.0830**	0.5067	**0.5042**	0.0470	**0.0365**	0.1032	**0.0869**
T.E. (Best)	0.2988	**0.2611**	0.4355	**0.3848**	**0.0697**	0.0985	**0.0536**	0.0719
T.E. (Worst)	0.3076	**0.2695**	0.4417	**0.3929**	**0.0890**	0.1317	**0.0651**	0.1159
T.E. (Avg.)	0.3011	**0.2645**	0.4387	**0.3897**	**0.0793**	0.1108	**0.0591**	0.0909

From the smaller data sets, I (Iris) and II (Wine), it is obvious that the ABSOM has lower values of the QE, TE indices not only the best but also the worst and average parts.

From the larger data sets III and IV, however, the ABSOM has all lower values of the QE but higher values of the TE. Although the performances of the two algorithms on QE and TE are not identical, we found the ABSOM always has better DB index value no matter what is the size of the data sets. As we know, the QE index is more representative than the TE index to indicate the final result of a clustering analysis method. In addition, we found that the ABSOM on the performance of the QE indices as well as the concentration on the map topologies are all better than the SOM. The results can be explained because of the exploration strategy of the state transition rule. The ABSOM has the ability to jump out from local minima and find a better solution. For the aspect of TE index, it seems reasonable that the ABSOM with the capability of jumping out the local minima may select a map unit far away from the one which has the shortest distance with the input vector at the beginning, so that it gets different BMU and worsen the TE value in the two larger data sets if comparing with the conventional SOM.

To investigate the benefit of the ABSOM, the further examination techniques, U-matrix and block diagram of map topology, are conducted for both the algorithms. The U-matrix can facilitate the identification of the boundaries for different clusters; the block diagram of map topology shows the number of data mapped on each output unit which can also ease the identification of different clusters and their centers. In the block diagram method, since the size and color of a block respectively represent the number of data mapped on the corresponding map unit and the cluster belonged, the bigger size of blocks stands for the larger number of data mapped on the corresponding map units. Using the previous four data sets with the given solutions, the ABSOM and SOM obtain the final results shown on the network topology by the U-matrix method and the block diagram method.

As shown in Fig. 2, the map topologies from the SOM and ABSOM are all quite different. For example, the data distribution of each cluster sometimes is quite different from these two algorithms. Taking the iris data set for example, the first cluster (represented by red color) formed by the SOM is located on the lower part of the map in Fig. 2, but the first cluster formed by the ABSOM is located on the right bottom corner of the map. If we show the results from the U-matrix and the block diagram on a map topology, it seems much clear that the ABSOM can get a different and better solution under the same initial weight vectors.

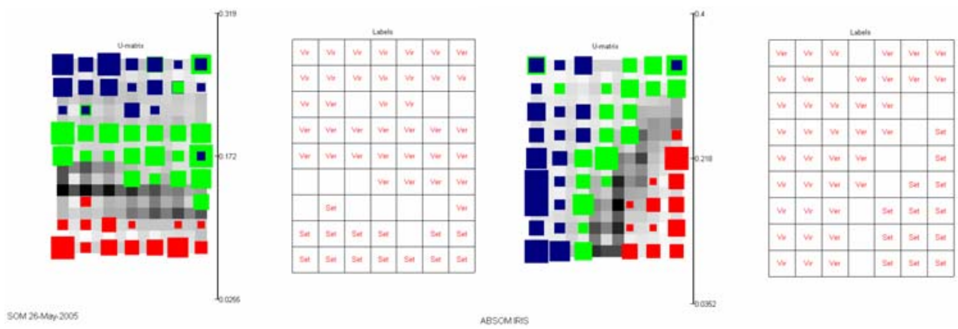

Fig. 2 Visualization of Map topology from the SOM (left)/ABSOM (right) for Iris data set

5 Conclusion and Future Work

In summary, this research has proposed an new algorithm named the ABSOM, that combines the ant colony system with the Kohonen's SOM, to overcome the local minimal issue on the Kohonen's self-organizing maps. In this research, We compared the ABSOM with the conventional SOM using four data sets with the given solutions and finally we found out the ABSOM is superior to the conventional SOM in general.

As pointed by recent researches, the fixed structure of the conventional SOMs can not afford to respond the real data distribution if the original data set consists of vague boudaries of different clusters. Therefore, our research work will extend the proposed ABSOM approach to create a growable ant-based SOM for solving this kind of problem.

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