Refining the Scatteredness of Classes using Pheromone-Based Kohonen Self-Organizing Map (PKSOM)

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Abstract— **The Kohonen Self-Organizing Map (KSOM) is one of the well-known unsupervised learning algorithms, which has been applied in various areas. This algorithm can cluster and classify an enormous amount of data into several clusters according to the similarity of the data features. However, it has many drawbacks, such as difficulty of clustering the data, which have similar features. These may lead to the inefficient result; the data is scatteredly mapped even though it is accurately clustered into several clusters according to the features. Therefore, this paper proposed a Pheromone-based Kohonen Self-Organizing Map (PKSOM) algorithm to refine the scatteredness of the data in the clusters, thus to improve the cluster density. Some modifications have been made to the original Kohonen Self-Organizing Map (KSOM), adapted from the Ant Clustering Algorithm procedures. This PKSOM has been tested on three different datasets; Iris flowers, Glass and Wood datasets. Based on the result, the proposed method has improved the classification impressively by increasing the density of the data in clusters. Hence, it has also refined the scatteredness of classes, where each dataset is well clustered where data that have similar features are located closely to each other in the same cluster. However, there are a few overlapped clusters that still occur.**

Keywords–Kohonen Self-Organizing Map (KSOM); Pheromone; Ant Clustering Algorithm (ACA); Clustering; Cluster density.

I. INTRODUCTION

The Kohonen Self-Organization Map (KSOM) is an unsupervised learning technique that is expended by topological self-organizing maps stemming from techniques that were first proposed for competitive learning [1]. This algorithm is used to process the high dimensional data, and it is also designed to cluster the data into clusters of data that exhibit some similarities. Each cluster with similar features is projected onto the same node on the map. Otherwise, the dissimilarity increases with the distance that separates two projections on the map. Thus, the cluster space is identified to the map, so that the projection enables simultaneous visualization of the cluster and the observation space [2]. Being one of the most popular unsupervised learning technique, KSOM has been used in different areas, in clustering, that might help to solve a complex problem. Giraudel et al. [3] discussed a comparison between the application of KSOM and other conventional ordination methods for ecological community. As mentioned earlier, KSOM has been used in different areas for many purposes. Anthony has used the KSOM to develop a new color quantization algorithm for mapping the 24-bit color images to eight-bit color [4]. They proved that their proposed algorithm could produce better output compared to the Oct-Tree and Median-Cut algorithms with very limited samples. While Emamian et al. [5] have proposed the application of KSOM to recognize the transient crack-related signals in the presence of strong time-varying noise and other interferences. The application can cluster the acoustic emission signals for fault monitoring and as a result, it is showed that the KSOM did perform well with a small probability of error.

The KSOM has also been widely used as a visualization tool for dimensionality reduction. Its unique topology preserving property can be used to visualize the relative mutual relationships among the data. It has been applied to organize and visualize vast amount of textual information, for example, the SOM that organizes massive document collection; WEBSOM [6]. The main benefit of KSOM is the topology preservation of an input space, which makes similar object appear closely on the map. Most of these applications, however, are based on 2D grids and map. Weijian et al. [7] investigated a hybrid neural network framework by combining the supervised learning algorithm with unsupervised algorithm on integrated representation platform of multiple two dimensional KSOM with the assistance of associative memory for clustering and classification of Remotely Sensed (RS) imagery. The formation of the clusters and the transformation from clusters to decision regions are implemented by unsupervised and supervised self-organizing learning on several Kohonen 2D Self-Organizing Maps (M2dSOM), individually. Xu et al. [8] used the two important operations in KSOM: vector quantization and topological preserving mapping, while introducing an online Self-Organizing Topological Tree (SOTT), with faster learning, is proposed. Their proposed learning rule is novel and delivers the efficiency and the topological preservation compared to other structures of KSOM. The computational complexity of

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SOTT is better and its computation time is much shorter than the entire search process done by KSOM. Forkan et al. [9] proposed a new method for surface based on hybrid techniques using KSOM and Particle Swarm Optimization (PSO). The KSOM learns the sample data through mapping grid. Consequently, the learned and well-represented data has become the input for surface fitting procedure. The authors have proposed PSO to probe the optimum fitting points on surfaces and this algorithm has been applied on different types of curve to observe its ability in reconstructing the object while preserving the original shapes.

However, the KSOM has several weaknesses, such as the difficulty of clustering and classifying the data, which have similar features, and this may lead to an inefficient result. Therefore, to improve the clustering result, a few researchers have proposed an optimized Kohonen by hybridizing KSOM with other techniques such as K-mean [19], simulated annealing [20], rough set theory and genetic algorithm [21], and Ant Colony Optimization (ACO) [22][23].

There are numerous researches have been conducted using the combination of KSOM with ACO for clustering. For example, Mora et al. [22] proposed an ant-based method that takes benefit of the cooperative self-organizing ACO named as KohonAnts. It is designed as a clustering algorithm that is capable of grouping a set of the input samples into clusters with similar features same as KSOM behavior. The data is grouped without considering the class of the input pattern during the process. While Yang et al. [23] also applied ACO in their Ant-based of Self-Organizing feature Maps algorithm (ABSOM). This algorithm utilized the pheromone mechanism of ant colony system to memorize the history of the best matching unit and also adopted the state of transition rules of exploitation and exploration in ACO to determine the best matching unit. Chen et al. [27] proposed a new clustering method named AMC algorithm that can be accelerated by the use of a global memory bank, increase the radius of perception and also a density-based method that permits each ant to look for objects. This algorithm has reduced the times of region inquiry, hence, saved the clustering time.

Even though most of these hybrid algorithms are capable of grouping the data samples accurately into required classes, unfortunately the data samples are scatteredly mapped on the topology map. Moreover, it is hard to identify the separation boundary among the classes. Therefore, this paper has proposed a Pheromone-Based Self-Organizing Map (PKSOM) algorithm to refine and improve the scatteredness of the data in the clusters by modifying the KSOM algorithm using the pheromone concept from the Ant Clustering Algorithm (ACA). The ACA is chosen because of its strength, where it is robust, flexible, self-organize, good convergence and parallel [24]. It is a probabilistic technique for solving computation problem, which can be reduced to finding a good path through graph [25]. Besides, it can cluster the data samples into numbers of clusters and the total number of cluster is generated automatically [26].

This paper has been organized as follows. After presenting all concepts used in our method, in section Data Clustering, then we will discuss the proposed methods thoroughly, followed by a discussion on experimental works and analysis of results. Finally, we will conclude out description in the last section with a discussion of the obtained results and future works.

II. Data Clustering

A. Kohonen Self-Organizing Map (KSOM)

Developed by Teuvo Kohonen in year 1982, Kohonen Self-Organizing Map (KSOM) is an example of unsupervised training method for neural networks that implements the vector quantization [6]. Differing from the traditional vector quantization where KSOM task is to define how the mapping, m is ordered and how the input x is distributed on the map. In KSOM, there are a few factors that might influence the clustering results such as learning parameters, topology map and map sizes. The major steps in KSOM are in the distance calculation and the weights update. A KSOM unit computes the Euclidean Distance between an input x and its weight vector w. In the Kohonen one-dimensional network, the neighborhood of radius 1 of a unit at the k^{th} position consists of the units at the positions $k - 1$ and $k + 1$. The KSOM network and its algorithm are shown in Fig. 1 and Fig. 2.

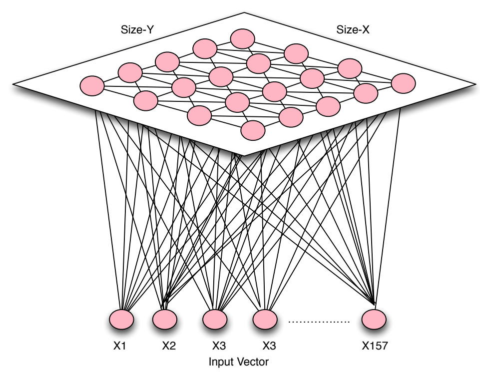


Figure 1. The KSOM network.

The performance of KSOM algorithm is measured using two measurements that commonly used in evaluating and measuring the self-organization algorithm: topological error and quantization error [10]. The topological error is used to measure the proportion of all data vectors for which first and second-best matching unit or winning unit are not adjacent vectors. If the value of topological error is lower then the KSOM preserves the topology is better. The quantization error is used to measure the average distance between each data vector and its best matching unit or winning unit. If the value of quantization error is small then it shows that the input vector is closer to its prototype.

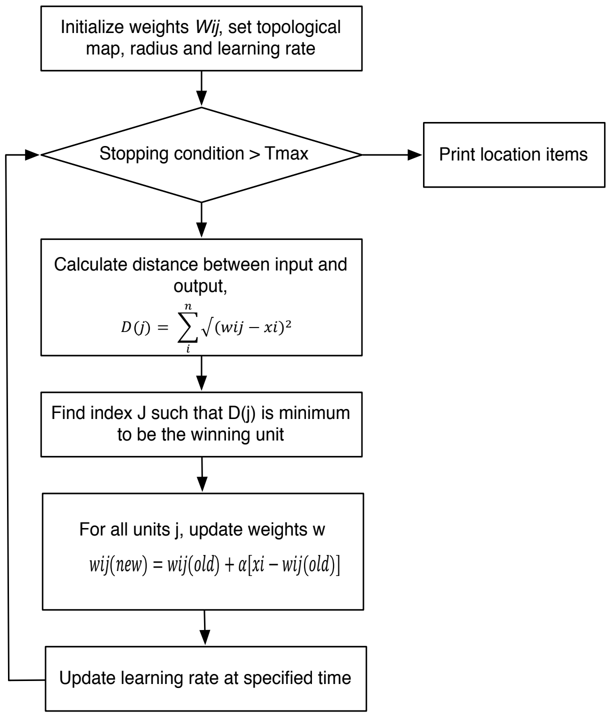


Figure 2. The KSOM Algorithm

B. Ant Clustering Algorithm (ACA)

The Ant Clustering Algorithm (ACA) [16] is an ant colony optimization algorithm that is designed for clustering purposes. It is a self-organizing algorithm where, the positive and negative feedback can display sudden modification that affect the pattern at the global level and the interaction is based on the cues and signals. Artificial ants are needed and the movements of these ants are based on the probabilities to pick up and drop down the object that are inversely proportional to the number of objects that are has experiences within a short period. Therefore, the ant will be more likely to deposit the object near larger clusters of objects. This algorithm applied the similarity idea where the degree of pair of data objects can reveal their probability of grouping into the same cluster. Fig. 3 shows the algorithm for ACA by Lumer et al. [11].

The ant can measure the similarity of the objects perceived within a local region and also identify the objects at the central site that is equally likely to group with the other objects. This algorithm used two types of pheromone for its searching strategy: cluster pheromone and object pheromone. Normally the cluster pheromone is used to lead or guide the ant to search for compact clusters while the object pheromone is to guide the ant to search for an object to be picked up and dropped. Both picking and dropping decisions require the evaluation of *f(i)*, which provides information on the similarity and density of the data items in the ant's local neighborhood.

```
procedure LUMER & FAEITA
Randomly scatter data items on toroidal grid
Randomly place agents on the toroidal grid
for t=1 to max iterations do
  j=random agent
  move agent j randomly by step size grid cells
  l= is agent j's grid position occupied by data item?
  e= is agent j's grid position occupied by a data item?
  if(l=TRUE) AND (e=FALSE) then
  i=data item carried by agent j
  drop=(random()<=pdrop(i)
  if drop = TRUE then
let agent j drop data item i at its current post
  end if
end if
if (l=FALSE) and (e=TRUE) then
  i=data item at agent j's grid position
  pick=random()<=Ppick(i)
  if pick=TRUE then
  let agent j pick up data item i
  end if
end if
end for
end procedure
```

Figure 3. The Ant Clustering Algorithm (ACA) algorithm

III. PHEROMONE-BASED KOHONEN SELF-ORGANIZING MAP (PKSOM)

The proposed algorithm; Pheromone-Based Kohonen Self-Organizing Map (PKSOM) is a modified KSOM using a pheromone concept adapted from the ACA algorithm. As mentioned before, there are two main steps in KSOM that determine the self-organizing process: (1) distance calculation and (2) weight update. Some modification has been made to these two steps using the pheromone concept. The full PKSOM algorithm is shown in Fig. 4.

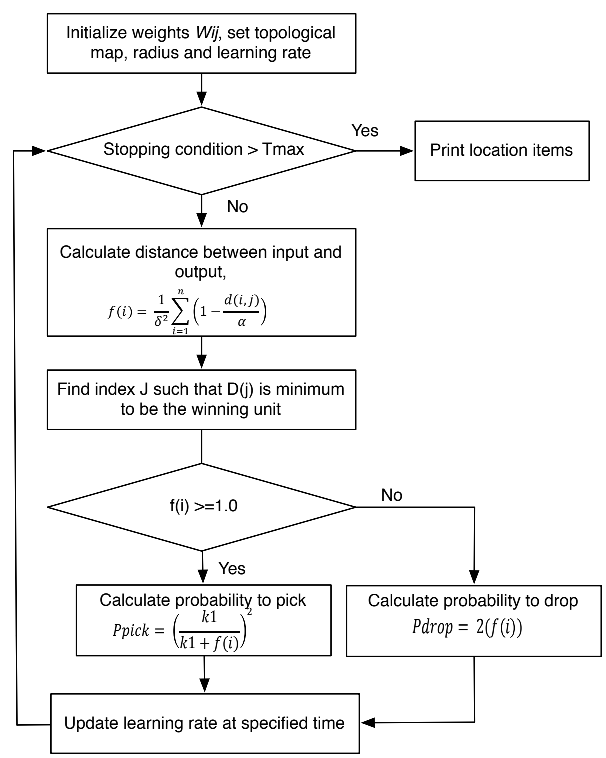


Figure 4. The PKSOM Algorithm

A. Distance Calculation

In KSOM, the distance calculation uses Euclidean Distance (ED); a distance between two points on a plane. The calculation is shown in (1) [1].

$$d(j) = \sum_{i=1}^{n} \sqrt{(wij - xi)^2} \quad (1)$$

The w_{ij} is representing the weight connection between input and output node, while x_i is the value of input *X*. This equation compares two objects across a range of variables and determines how dissimilar the objects are. In KSOM, the minimum value of ED is selected to be a winning unit. The minimum value also shows the two objects are very similar to each other.

For modification, the ED is replaced using Pheromone Density Measure (PDM) in ACA, as shown in (2). The pheromone density function is a way to measure the average of the similarity of objects o_i and other objects present in the neighbor δ, instead of looking at the distance, individually [11].

$$f(i) = \frac{1}{\delta^2} \sum_{i=1}^{n} \left(1 - \frac{d(i,j)}{\alpha}\right) \quad (2)$$

Here, the *d(i,j)* is to define the distance or dissimilarity between objects in the space of objects' attributes. While the α is a discriminant factor that defines the scale of dissimilarity and it is important for it to determine when two items should be or should not be located next to each other. The value selection for α is also crucial where this might affect the formation of clusters. If the α value is too large, there might not be enough discrimination between different items that may lead to the formation of clusters composed of item, which should not belong to the same cluster. On the other hand, if the value is too small, the distances between items in the space are amplified to the point where the items, which are relatively close in attribute space cannot be clustered together because the discrimination is too high.

B. Weights Update

Despite the pheromone density calculation, the other modified step is the weights' update. In original KSOM algorithm, the weight changes are calculated using Gaussian function [2], as shown in (3). The Gaussian function is used as a decreasing function of the grid distance between objects. Due to the collective learning scheme in KSOM, the input signals, which are near to each other, will be mapped on neighboring neurons. Thus, the topology inherently present in the input signals will be preserved in the mapping. The *rk* and *rc* represent the two objects to be calculated, while the δ is representing the neighborhood radius.

$$\Delta w = exp\left(-\frac{(rk - rc)^2}{2\delta^2}\right) \quad (3)$$

In order to ensure this algorithm works well with pheromone density calculation, the Gaussian function is replaced with the probability to pick up (4) and probability to drop (5) the object in ACA. Deneubourg et al. [17] have proposed these probabilities based on the corpse clustering and the larvae sorting in ants; where the isolated item should be picked up and dropped at some other location where more items of that type are present. The decisions to drop and pick the object are random and influenced by the data items in the neighborhood. The probability of dropping an item might increase if the surrounded neighborhood data is similar. In contrast, the probability of picking an item might increase if the surrounded neighborhood is dissimilar.

$$Ppick = \left(\frac{k1}{k1 + f(i)}\right)^2 \quad (4)$$

$$Pdrop = \begin{cases} 2(f(i)\ when\ f(i) < k2 \\ 1\ when\ f(i) \geq k2 \end{cases} \quad (5)$$

For both equations, the *f(i)* is the PDM, while the k_1 and k_2 are threshold constants. The selected value for both *k* is 1 and this is according to Lumer et al. [11], where they have defined a distance or dissimilarity between objects in the space of object attributes:

- If two objects are similar or identical, then the $d(o_i,o_j) = 0$
- If two objects are not similar or identical, then the $d(o_i,o_j) = 1$

IV. EXPERIMENTAL WORKS AND ANALYSIS OF RESULTS

A. Experimentals Works

The proposed algorithm has been tested using three different datasets; (1) Iris, (2) Glass and (3) Wood datasets (as shown in Table 1). The Iris dataset consists of 150 samples, which represent 3 species; sentosa, virginica and versicolor. While for Glass's data, the dataset has 216 samples and can be categorized into 2 categories; window and non-window glass. Moreover, the dataset for Wood that owned 5040 samples of data comprises 52 tropical Wood species and this dataset can also be categorized according to the most dominant features; the pore size. There are three sizes of pores; small, medium-sized and large and the list of tropical wood species based on pores sizes is shown in Table 2.

TABLE 1: THE DATASET USED TO EVALUATE THE ALGORITHM

Datasets	No of Samples	Attributes	Category
Iris	150	4	3
Glass	215	9	2
Wood	5040	157	3

TABLE 2. TROPICAL WOOD SPECIES BASED ON PORES SIZES

Pore Sizes	Wood Species
Small	mataulat
Medium-Sized	balau, bintangor, bitis, chengal, gerutu, giam jelutong, kapur, kasai, kekatong, keledang, keranji, kulim, machang, medang, melunak, perupok, redbalau
Large	bintangor, durian, gerutu2, kapur, kasai, keledang, keruing, machang, merantibakau, redbalau, rubberwood, sesendok

The training processes are done repetitively and each dataset used different parameters; such as learning rate and number of epochs. These values have been personalized to each dataset and parameters values are obtained from the KSOM training process for performance comparison purposes. Table 3 shows the full parameters used for these three datasets. The selection of topological map for all datasets is based on Alhoniemi et al. [18], calculated using:

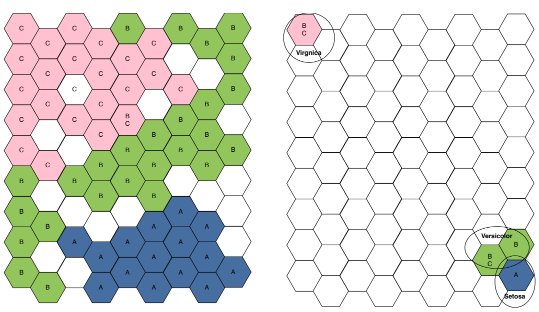
$$mapsize = 5(\,no\ of\ sample^{\,0.54321}) \quad (6)$$

TABLE 3. FULL PARAMETERS USED FOR ALL DATASETS

Parameters	Datasets		
	Iris	Glass	Wood
Topological Map	9x9 (81 nodes)	9x9 (81 nodes)	23x23 (529 nodes)
Sample number	150	216	5040
Categories/ Number of Clusters to be clustered	3 (Setosa, Versicolor & Virginica)	2 (Window-Glass & Non-window Glass)	3 (Small, Medium-sized & Large pores)

B. Results

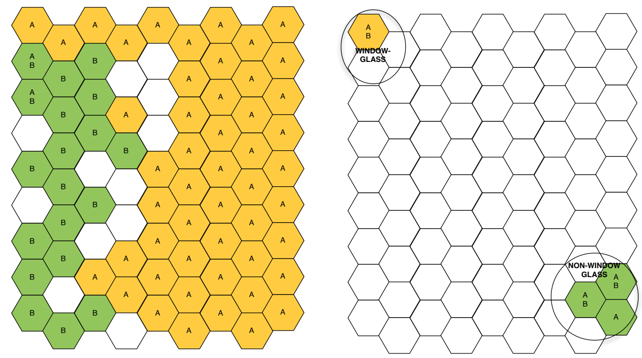
As a result, it is obviously seen that the PKSOM has improved and refined the scatteredness of clustering data by increasing the density of the data in clusters. Most of the data are well clustered and closed to each in the same cluster even though there is a few dislocated data occurred and performed the overlapped clusters. Fig. 5 shows the results for Iris dataset using both algorithms. KSOM has clustered the Iris dataset into three big clusters (consists of a few clusters for every species) according to the species. However, the PKSOM has also clustered the dataset into three different clusters with high density of data in each cluster.



(a) (b)

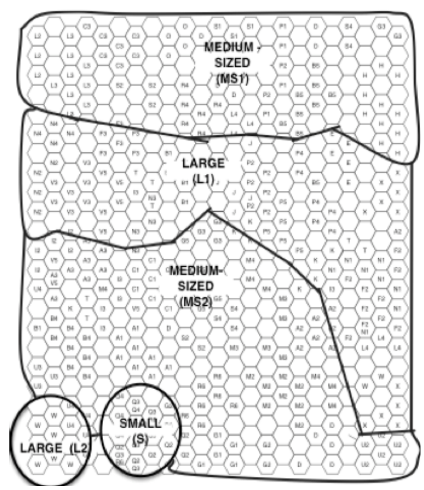
Figure 5. Clustering Results using (a) KSOM and (b) PKSOM for Iris Dataset

Fig. 6 shows the clustering results performed by KSOM and PKSOM for Glass dataset, where the KSOM has separated the dataset into two categories: the window glass (on the upper part of the map) and non-window glass (on the lower part of the map). Conversely, the PKSOM has clearly separated the dataset into two different classes with a minimum number of cluster nodes and high density of data in each node. While for Wood dataset, KSOM has clustered the whole dataset into five big clusters: one cluster for small pores, two clusters for medium-sized pores and two clusters for large pores. However, the PKSOM has clustered the Wood dataset into three desired clusters, accurately. This is shown in Fig. 7.

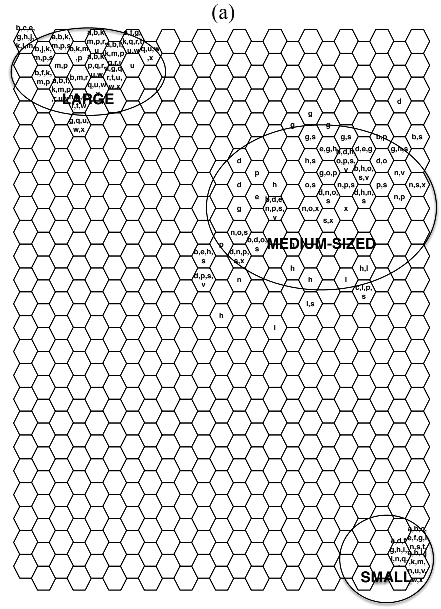


(a) (b)

Figure 6. Clustering Results using (a) KSOM and (b) PKSOM for Glass Dataset



(a)



(b)

Figure 7. Clustering Results using (a) KSOM and (b) PKSOM for Wood Dataset

TABLE 4: FULL RESULT FOR ALL DATASET

Dataset	Map Size	Cluster Usage (Cluster Node With data)		Average Cluster Density of single node	
		KSOM	PKSOM	KSOM	PKSOM
Iris	9 x 9 (81 cluster nodes)	64	4	±2	±38
Glass	9 x 9 (81 cluster nodes)	69	4	±3	54
Wood	23 x 23 (529 cluster nodes)	399	71	±13	±71

Conclusively, as shown in Table 4, the KSOM has clustered Iris dataset into 64 clusters, Glass dataset into 69 clusters and wood dataset into 399 clusters. The percentage of cluster usage (the cluster node that consists of data) for Iris dataset is 79.01%, Glass dataset is 85.19% and for wood dataset is 75.43%. While for proposed algorithm, PKSOM, the percentage of cluster usage for every dataset are 4.94% (Iris dataset), 4.94% (Glass dataset) and 23.92% (wood dataset), as shown in Fig. 8.

Even though the KSOM's average of cluster usage is higher than the PKSOM, but the average cluster density of each cluster is lower compared to PKSOM (shown in Fig. 9). The PKSOM has the produced high average cluster density for every dataset; for Iris, the average cluster density is 38, Glass dataset average cluster density is 54 and for wood dataset is 70.99. However, the average cluster densities for every dataset produced by KSOM are very low; 2.34 (Iris dataset), 3.13 (Glass dataset) and 12.63 (Wood dataset).

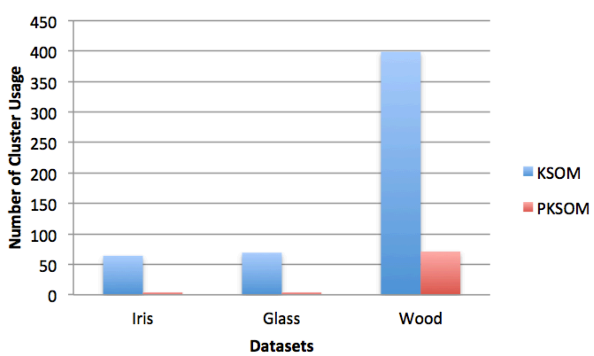


Figure 8. The Difference of Cluster Usage between KSOM and PKSOM

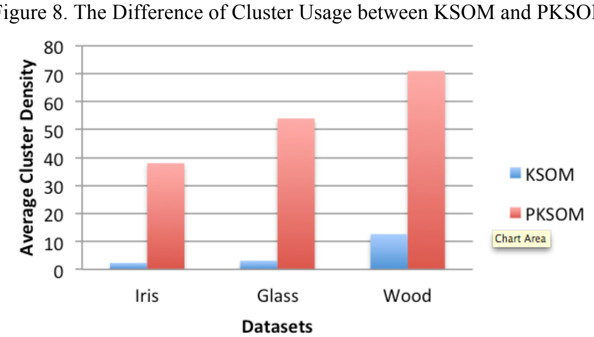


Figure 9. The Average Cluster Density of single node

For performance evaluation, we have compared the PKSOM result with previous methods; KohonAnts [22] and ABSOM [23] based on Iris results. Fig. 10 shows the results for KohonAnts, ABSOM and PKSOM. Both methods: KohonAnts and ABSOM have produced good classification result but the clustered data is scatteredly mapped into a two dimensional map. However, it is clearly seen that PKSOM has clustered the Iris dataset into three clusters, same as KohonAnts and ABSOM but with a minimum number of cluster usage. This is proved that PKSOM has refined the scatteredness of the data, thus improved the separable boundary between clusters.

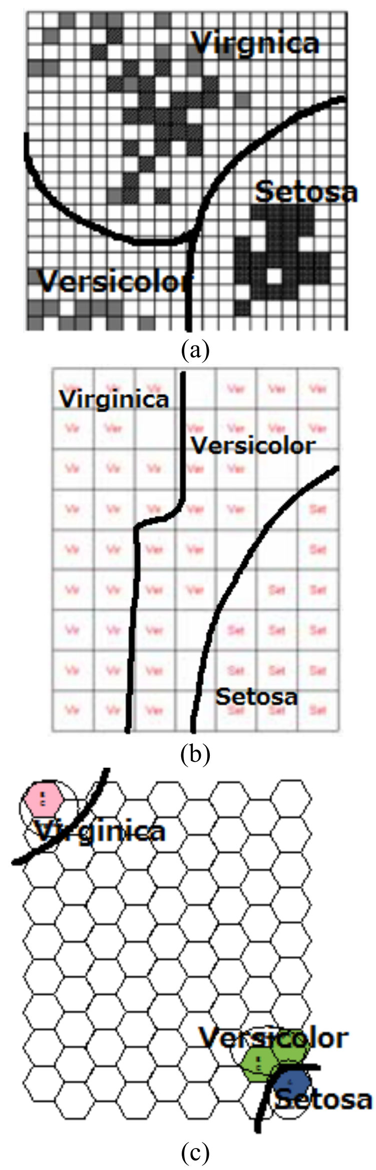


Figure 10. Clustering Results using (a) KohonAnts, (b) ABSOM and (c) PKSOM for Iris Dataset

V. CONCLUSION AND FUTURE WORK

In conclusion, it is obviously seen and proven that the PKSOM has improved and refined the scatteredness of clustering data by increasing the density of the data in clusters. Most of the data for all datasets are well clustered and closed to each other in the same cluster. However, there are a few dislocated data that performed the overlapped clusters. These overlapped clusters consist of at least two different species or category in every overlapped cluster. According to the result, also, we can conclude that PKSOM also can deal with high dimensional dataset, such as wood dataset. Furthermore, we will perform further test using different high dimensional and sparse dataset to investigate the effectiveness of the proposed method. In addition, we will make some refinement to the algorithm in order to solve overlapped clusters problem and increase the classification accuracy.

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