Dimensional Reduction and Data Visualization Using Hybrid Artificial Neural Networks

Chee Siong Teh, Ming Leong Yii, and Chwen Jen Chen

***Abstract*—Data with dimension higher than three is not possible to be visualized directly. Unfortunately in real world data, not only the dimension are often more than three, very often real world data contain temporal information that makes the data only useful and meaningful when they are interpreted in sequence. Dimensionality reduction and visualization techniques such as self-organizing map (SOM) are usually used to explore the underlying multidimensional data structure. However, SOM only preserves inter-neurons distances in the input space and not in the output space due to the rigid grid used in SOM. Visualization induced self organizing map (ViSOM) was proposed as an extension of SOM in order to preserve the output space topology. In this paper, the modified adaptive coordinates (AC) technique is proposed to improve the visualization of SOM without the need to increase the number of neurons as in ViSOM. With a better visualization map formed, a post-processing technique is incorporated into the algorithm to produce a hybrid that is capable to extract temporal information contained in the data. Empirical studies of the hybrid techniques yield promising topology preserved visualizations and data structure exploration for synthetic and benchmarking datasets.**

***Index Terms*—Adaptive coordinates, artificial neural networks, spatial-temporal multivariate data visualization, multi-dimension reduction.**

I. Introduction

Visual information is essential for human intuitive decision making. Data with dimension higher than three, which we often found in natural occurrences, is not possible to be visualized directly. Real world data such audio-visual recording, geographical sensors tracking, and stock market, not only they consist of large and growing in dimensions, very often the data is temporally connected between samples. These spatial-temporal data, can only be visualized and interpreted in sequence through the use of dimensionality reduction techniques that take sequence into account.

Classical method such as Sammon’s Non-linear Mapping (NLM) [1] and Multidimensional Scaling (MDS) [2] provide excellent ways in dimension reduction. But these techniques have two major drawbacks. First, due to their point-to-point mapping nature and calculation complexities, they are not practical for real life applications where databases are always expanding.

Algorithms with data compression or vectors quantization and visualization abilities are more preferable in real life applications. Self Organizing Map (SOM) proposed by Kohonen [3] is far better for real-world applications. However, both the classical method and the original SOM cannot process the temporal information that often contain in the sequence of that data.

SOM can be used for dimension reduction, vector quantization and visualization. Recent application of SOM in real life problems can be found in [4]-[7]. Although SOM has become a very popular analytical tool, it has one major drawback. Due to its rigid grid used in the output space, only the input space data topology is preserved. The output space of SOM is represented by a rectangular or hexagonal grid which does not preserve the inter-neuron distances. [8]-[11] pointed out this drawback and proposed new algorithms that preserve the inter-neuron distances in the output space.

Adaptive Coordinates (AC) was proposed as an extension to the original SOM [10], [11]. AC did not modify SOM, instead by using virtual adaptive units to mirror SOM neurons movement, AC is able to produce topology preserved output map. This is an advantage when compare with ViSOM in terms of the number of neurons utilized. The details of AC algorithm can be found in [10], [11]. Nevertheless, the projection ability of AC is very much depending on a magic number or free parameter that triggers the adaptation process. During initial training, the adaptation tends to be too strong and causes all adaptive units to move towards single point [11]. But if the adaptation starts too late, too little movement would be mirrored to produce meaningful visualization. This magic number can only be found heuristically. To lift this limitation, the original AC is modified and hybridized with SOM and ViSOM respectively for multivariate data dimension reduction and data visualization. This paper highlights this hybridization.

Visualization induced self organizing map (ViSOM) [8] was a more recent SOM’s extension proposed to overcome limitation of SOM. ViSOM tries to preserve the topological information in the output space like SOM does, as well as tries to preserve the inter-neurons distance through a regularization control parameter. ViSOM introduced a regularization control parameter so that the distances between two neighborhood neurons can be controlled. By regularizing the inter-neuron distances of the input space with suitable control parameter, the output space of the projected map is able to preserve the data topology. This control parameter defines the resolution of the map. Empirical results shows ViSOM is able to produce a more appealing visualization when compared with SOM. Nevertheless, extra underutilized neurons and longer training

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are the tradeoff for the better visualization. ViSOM requires larger number of neurons than SOM in order to produce a better visualization. Most of these extra neurons never get activated throughout the training. Large number of neurons increase computation cost and the projected map becomes more vulnerable to dead neurons problem as pointed out in [12], [13].

Section II gives an overview of SOM, ViSOM and original AC algorithms. The proposed hybrid of SOM with the modified AC (SOM-AC), and hybrid of ViSOM with the modified AC (ViSOM-AC) are presented in Section III. Section III also introduces a post-processing technique of the hybridized projection that capture the temporal information contained in the spatial-temporal data. Experiment results on synthetic and benchmarking dataset are presented in Section IV. This is followed by an application of the hybrid on a speaker identification problem. The results are analyzed and discussed in terms of visualization of the underlying data structure. Concluding remarks are presented at the end of the paper.

II. SOM, ViSOM and Original AC

A. Self-Organizing Map (SOM)

Kohonen's self-organizing map (SOM) [3] has the desirable property of topology preservation, which captures an important aspect of feature maps in the cortex of highly developed animals' brains. It is widely used for the projection of multivariate data, density approximation, and clustering. It has been successfully applied in many areas including speech recognition, image processing, robotics, telecommunication, and process control [3]. SOM network architecture basically consists of a two-dimensional array of units, each connected to all n input nodes with weights vector $\mathrm{w}_j = (w_{j1}, w_{j2}, ..., w_{jd})$ where d is the dimension of the dataset being analyzed. The learning process of SOM involved finding the Best Matching Unit (BMU), *i**, for each sample *x* drawn from dataset, using Euclidean norm

$$i^* = \arg\min_i \quad \|x - w_j\| \tag{1}$$

and updates the weights of all the connections according to the unsupervised "on-line" competitive learning rule

$$w_j(t+1) = w_j(t) + \eta.h_{i*j}(t)[x(t) - w_j(t)] \tag{2}$$

where η is the learning rate and $h_{i*j}(t)$ is the Gaussian neighborhood function

$$h_{i*j}(t) = \exp(-(r_{i*} - r_j)^2 / 2\sigma(t)^2) \tag{3}$$

$(r_{i*} - r_j)$ is the distance between BMU *i** and neuron *j* and

$$\sigma_{\wedge}(t) = \sigma_{\wedge_0} \exp(-2\sigma_{\wedge_0}(t / t_{\max})) \tag{4}$$

is the neighborhood range with initial value $\sigma_{\wedge_0}$ which is initialized with the half of the SOM lattice size.

Although SOM provides good input space topology preservation, the SOM map gives little intuitive information about the data topology due to the rigid predefined rectangular or hexagonal grid on the output space. SOM grid does not preserve the data topology.

B. Visualization-Induced Self-Organizing Map (ViSOM)

The basic idea behind ViSOM [8] is to regularize the lateral movement of neighborhood neurons during SOM updates so that the inter-neuron distances are preserved in the output map. The projection therefore becomes a smooth net (mesh) embedded in the N-dimensional data space. ViSOM decomposes the second term of SOM's update learning rule $x(t) - w_j(t)$ into two parts;

$$x(t) - w_j(t) = [x(t) - w_{i*}(t)] + [w_{i*}(t) - w_j(t)] \tag{5}$$

The update force can be rewritten as $F_{jx} = F_{i*x} + F_{ji*}$ where F_{i*x} is the force pulling the winner neuron towards input sample $\boldsymbol{x}$ and F_{ji*} is the lateral force that pulls neighborhood neurons *j* towards the winner neuron *i**. So, by constraining the lateral force F_{ji*} of the neighborhood through a multiplying coefficient $(d_{i*j} - \lambda\Delta_{i*j}) / \lambda\Delta_{i*j}$, the inter-neuron distances can be preserved. d_{i*j} and Δ_{i*j} are the inter-neurons distance in the data space and grid units respectively. λ is a free parameter introduced to ViSOM that controls the resolution of the projected map. The ViSOM weights update learning rule for neighborhood neurons becomes

$$w_j(t+1) = w_j(t) + \eta.h_{i*j}(t) \begin{pmatrix} [x(t) - w_{i*}(t)] \\ +[w_{i*}(t) - w_j(t)](d_{i*j} - \lambda\Delta_{i*j}) / \lambda\Delta_{i*j} \end{pmatrix} \tag{6}$$

C. Adaptive Coordinates (AC)

The Adaptive Coordinates (AC) [9] was proposed to remove the rigidity of SOM grid map, thus allowing a more intuitive recognition of the input data cluster boundaries. The basic idea of AC is to mirror the movement of neurons' weight vectors, in each of the SOM training iterations, into two dimensions adaptive coordinates $\langle ax_i, ay_i \rangle$. For each iteration *i*, the distances between neurons weights before SOM's weight vectors adaptation $Dist_i(t)$ and after the adaptation $Dist_i(t+1)$ are used to compute the relative AC adaptation factor.

$$\Delta Dist_i(t+1) = \frac{Dist_i(t) - Dist_i(t+1)}{Dist_t(t+1)} \tag{7}$$

The adaptive coordinates, except the winner node, is then moved towards the winner neuron *c* according to the equations as follows:

$$\begin{aligned} ax_i(t+1) &= ax_i(t) + \Delta Dist_i(t+1) \cdot (ax_c(t) - ax_i(t)) \\ ay_i(t+1) &= ay_i(t) + \Delta Dist_i(t+1) \cdot (ay_c(t) - ay_i(t)) \end{aligned} \tag{8}$$

As highlighted in [12], [13], AC suffers from inconsistent adaptive units movements due to the use of relative adaptation factor as shown in (4). The initial SOM training tends to be too strong and causes movements of the adaptive units to fall into a single point. Following that, when SOM is converging, there will be too little weight vectors movements to give notable mirroring movement of the adaptive units. It means that the remaining training epoch will not improve the visual projection on the AC after SOM is converged. It will simply waste the computational cost. This threshold value that triggers the starting of adaptation can only be found heuristically. This is not desirable because it reduces the robustness of SOM. Therefore to ensure a better visual projection on the AC and SOM, this study proposes a few approaches to modify the original AC.

III. The Proposed Hybrid Artificial Neural Networks for Spatial-Temporal Data Visualization

A. Proposed Hybridization of SOM and Modified AC (SOM-AC)

The original SOM algorithm is extremely robust. No parameter is required to produce good topological preserved map. But as highlighted in the previous section, SOM does not preserve the inter-neuron distance in the output space due to its rigid grid. A modified AC is proposed to remove this rigidity so that a better topology preserved map can be produced.

In order to successfully hybridized the modified AC with SOM while retaining the robustness of SOM, an extra set of coordinates $\langle ax_i, ay_i \rangle$ is used as the adaptive units. These adaptive units are used to mirror the movement of neurons. To overcome the inconsistent movements of these adaptive units for every iteration, the input and output spaces are normalized so that all movements are within the scale of 0 to 1. (9) shows the modified adaptation factor.

$$\Delta Dist_i(t+1) = d_{out}(t) - d_{in}(t) \tag{9}$$

where $d_{out}(t)$ is the Euclidean's distance of adaptive coordinates in the output space and $d_{in}(t)$ is the Euclidean's distance of the respective neurons weights. Instead of mirroring directly the movements of neurons as proposed in [10], the modified adaptation factor will approximate the distances of neurons and their respective adaptive units. The polarity of the adaptation factor will determine whether the adaptive coordinates will be pulled closer to the winner or pushed away from it through the coordinate update formula as in (10),

$$\begin{aligned} ax_i(t+1) &= ax_i(t) + \Delta Dist_i(t+1) \cdot \sigma_{\wedge}(t) \cdot (ax_c(t) - ax_i(t)) \\ ay_i(t+1) &= ay_i(t) + \Delta Dist_i(t+1) \cdot \sigma_{\wedge}(t) \cdot (ay_c(t) - ay_i(t)) \end{aligned} \tag{10}$$

where $\sigma_{\wedge}(t) = \exp(-2\sigma_{\wedge_0}(t / t_{\max}))$ is the adapted neighborhood range as in (4). Its value is exponentially decreasing between (0, 1). Since the proposed algorithm removes the need of a threshold to start the adaptation, the adaptation process will start after SOM is converged. This reduces the overall computational cost.

The proposed algorithm can be summarized as follows:

Step 1: Find the BMU for each sample that is selected according to (1)

Step 2: Update Codebook weights according to (2)

Step 3: Find the adaptation factor for a neuron according to (9)

Step 4: Update adaptive units according to (10)

Step 5: Repeat Step 1 to 4 according to a pre-defined number of epochs.

B. Proposed Hybrid ViSOM with Modified AC (ViSOM-AC)

ViSOM's topological and inter-neuron distances preserved map is produced at the cost of larger number of neurons. Most of these neurons never get activated. Modified AC as described in the previous section is therefore proposed to be hybridized with the ViSOM algorithm in order to alleviate this drawback. To overcome the inconsistent movement of AC during the training process, an adaptation factor as in Eq. (9) is used. Instead of directly mirroring the neurons weights movements as proposed in the original AC, it tries to preserve the inter-neuron distances from the *N*-dimensional neurons weights to the 2D adaptive units. The polarities of the adaptive factor will make the adaptive units move in bidirectional thus overcome the inconsistent movement of the original AC. Likewise, the adaptive units are updated using (10).

The proposed hybrid ViSOM with modified AC algorithm can be summarized as follow:

Step 1: Draw a random sample from a dataset

Step 2: Find winner according to (1)

Step 3: Updates winner and neighborhood neurons' weights according to (6)

Step 4: Find the adaptive factor according to (9)

Step 5: Adapt the AC units according to (10)

Step 6: Repeat Step 1 to Step 5 until stopping criteria is reached.

To further reduce the computational cost, Step 4 and 5 can be delayed until ViSOM starts converging which is around one fifth of the total training epoch.

C. Post-Processing SOM-AC for Spatial-Temporal Data Visualization

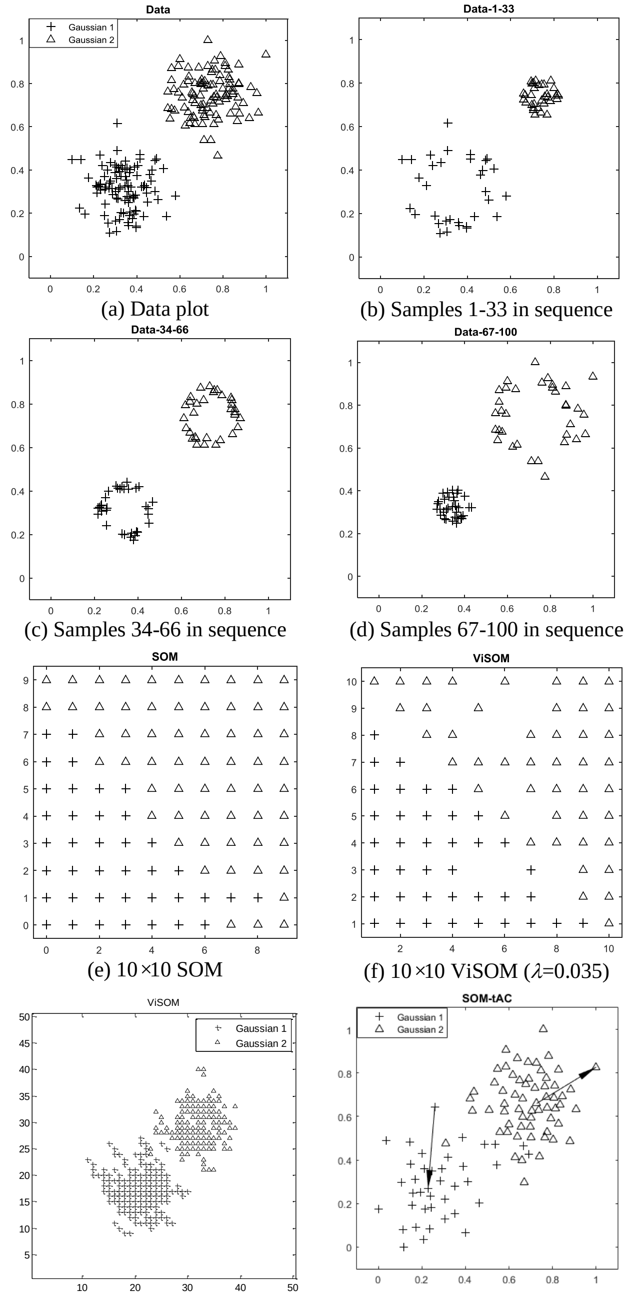
Post-processing technique is one of the three possible adaptations of SOM for temporal data processing [14]. No modification on the original algorithm is required. Instead, it can capture the progression of winner neurons as the data samples are fed sequentially into the network. By plotting the trajectory of the winners' neurons on top of the projected map, interesting information of the dynamic of the dataset is revealed. A prerequisite of a good post-processing temporal data projection is a good data projection of its relative spatial topology. Following section demonstrates how the hybrid produces intuitive visualization for spatial-temporal data.

IV. Experiments

The performance of the hybrid SOM with modified AC (SOM-AC) and hybrid ViSOM with modified AC (ViSOM-AC) are first demonstrated using synthetic 2D Gaussians datasets. 2D dataset is simple and can be visualized directly by human observer. Then benchmarking Wine dataset [10] is used to test the dimension reduction and topology preserved projection ability for higher dimension.

In all the experiments, the codebook vectors of SOM and ViSOM are initialized randomly, while the adaptive coordinates $\langle ax_i, ay_i \rangle$ are initialized with normalized values. For both SOM and ViSOM, the learning rate is set to be linearly decreasing from 0.35 to 0.01 for all experiments. Total training epoch number equals to 100, and initial σ value are equals to half of the lattice size. The ViSOM regularization parameter λ, otherwise mentioned, is set to 0.035 to control the resolution of the projected map.

A. Synthetic 2-D Gaussians



(a) Data plot (b) Samples 1-33 in sequence

(c) Samples 34-66 in sequence (d) Samples 67-100 in sequence

(e) 10×10 SOM (f) 10×10 ViSOM (λ=0.035)

(g) 50×50 ViSOM (λ=0.035) (h) 10×10 SOM with Modified AC

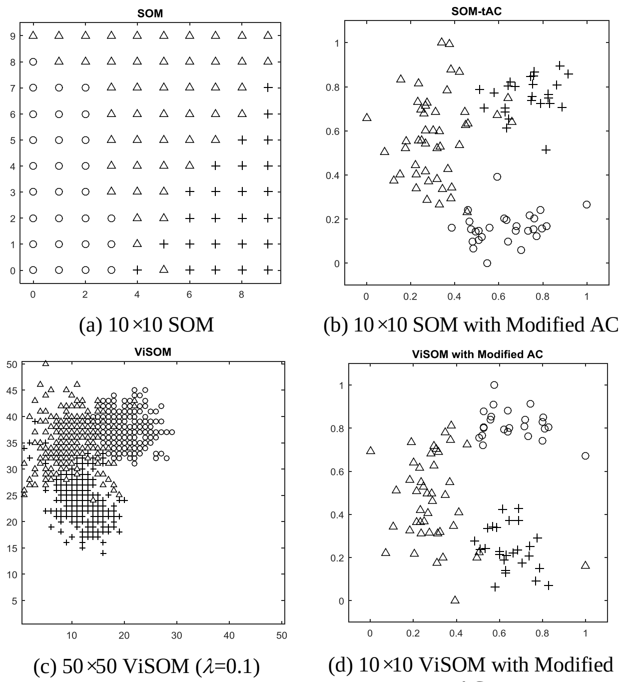
Fig. 1. The visualization of two synthetic 2-D Gaussians dataset.

The synthetic 2-D dataset consists of two well separated Gaussians with 100 samples each as shown in Fig. 1(a). Their mean vectors are 0.3 and 0.7 respectively. Fig. 1(b), (c), and (d) reveal another layer of information about the Gaussians; one is shrinking to its center and the other is growing from its center. Although both 10×10 SOM (Fig. 1(e)) and 10×10 ViSOM (Fig. 1(f)) clearly show two clusters of data, they contain little information regarding the data's underlying structure. Fig. 1(g) with 50×50 ViSOM shows a better visualization at the expense of higher processing cost due to the high number of neurons used. Hybrid SOM-AC improved this that with same 10×10 neurons, it is able to produce topology preserved output map in Fig. 1(h). On top of the projection, through the post-processing technique that track the trajectory of winners, the pointing arrows show the projection direction of the sequential movement for temporal data in Fig. 1(b) to Fig. 1(d). These provide very useful and intuitive information for potential user interaction.

B. Wine Benchmarking Dataset

Wine dataset [15] consists of 178 labeled samples with 13 dimensions and 3 different classes. Comparing with the previous datasets, this dataset has higher dimensions. SOM grid, as shown in Fig. 2(a), is able to reveal three different clusters after performing dimension reduction from 13D to 2D. Fig. 2(b) shows the intuitive information of the dataset and its clustering density are clearly depicted in the diagram.

ViSOM regularized visualization as shown in Fig. 2(c) shows three clusters in the map. However, it is still confined to the rigid grid. By removing the rigid grid through hybrid ViSOM-AC, visual inspection reveals three distinct clusters (see Fig. 2(d)). Both SOM-AC and ViSOM-AC provide better projections, even with much lower number of neurons, when compare with the ViSOM.



(a) 10×10 SOM (b) 10×10 SOM with Modified AC

(c) 50×50 ViSOM (λ=0.1) (d) 10×10 ViSOM with Modified AC

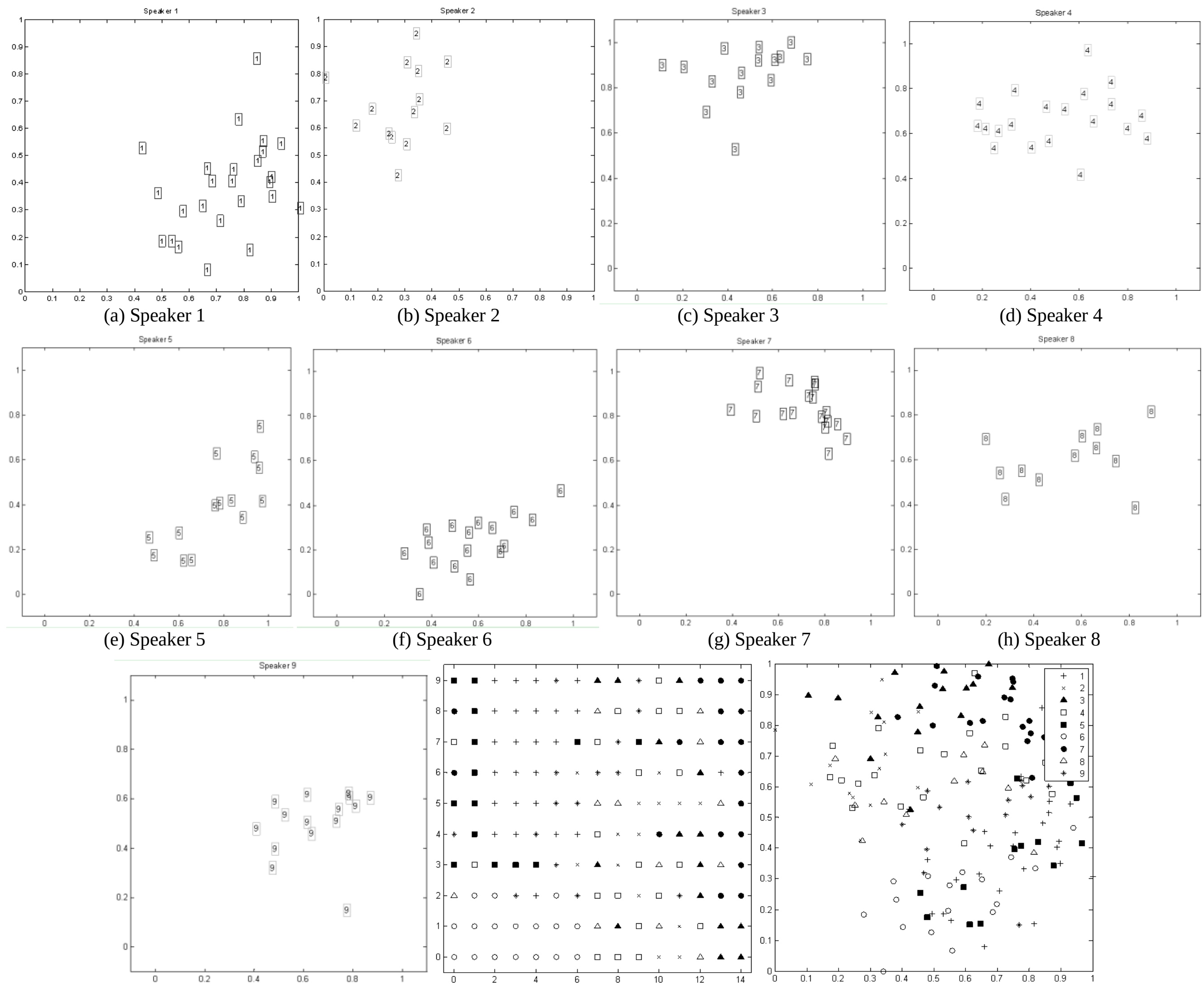
Fig. 2. 2-D visualization of wine dataset (13 dimensions, 3 classes).

V. Data Visualization in Speaker Identification Application

To demonstrate the usefulness of the hybrid algorithm in mining real-life multivariate time-series data, speaker identification of a real-value benchmarking dataset from UCI repository [16] was selected. This dataset consists of 640 time series taken from nine male speakers pronouncing Japanese vowel 'ae'. Each utterance was transformed and windowed into vectors of 12 LPC cepstrum coefficients. Different utterances consist of varying length between 7 to 29 vectors that are temporally connected. For classification task, 270 time-series was used for training and the remaining 370 for testing.

For the experiment setup 10×10 SOM was used with initial learning rate η=0.35 slowly decreasing to final value 0.01. Two phases of training were used to capture spatial-temporal information from the dataset. First phase disregards the sequence of data by feeding the samples randomly into the hybrid network for spatial information learning and projection. After the spatial map is formed, data is fed sequentially into the hybrid network to capture its temporal information in the second phase. This temporal information is useful for temporal pattern recognition and classification.

Fig. 3(a) to Fig. 3(i) show extracted clusters formed in SOM-AC that respectively represents the nine speakers' training data's spatial distribution. These clusters are visible but not distinct in 10×10 SOM visualization (Fig. 3(j)). Fig. 3(k) is the SOM-AC's overall visualization of the 9 speakers' 270 utterances. Interesting data structure and correlations between speakers, which was not available in SOM visualization, are revealed. Classification of the test data obtained 92.7% which is slightly behind reference accuracy 94.1% [17]. However, when the neuron size increases to 35×30, 96% classification accuracy was obtained. Further accuracy of 96.9% was obtained when both majority winners and winners' neurons trajectories are employed for classification.



(a) Speaker 1 (b) Speaker 2 (c) Speaker 3 (d) Speaker 4

(e) Speaker 5 (f) Speaker 6 (g) Speaker 7 (h) Speaker 8

(j) 10×10 SOM (i) Speaker 9 (k) 10×10 SOM-AC

Fig. 3. 2-D spatial visualization of 9 speakers' utterances.

VI. Conclusion

This paper proposes the hybridization of SOM-AC as well as hybridization of ViSOM-AC for data dimension reduction and data visualization. In the first experiment, the hybrid SOM-AC removes the rigid grid projection of SOM and thus produces a topological preserved map. Empirical results demonstrated the ability of such hybrid to produce promising data structure and inter-neuron distances preserved visualization as that in SOM. In the second experiment, the hybrid ViSOM-AC, taking all advantages offered by ViSOM, is able to produce informative and visually appealing visualization of a multivariate dataset. Fewer neurons are required by this hybrid model to produce quantized, dimensionally reduced, and topological and inter-neuron distances preserved visualization.

No predefined parameter is required for both types of hybridization. Therefore, the proposed hybrid techniques are useful in real life applications that require topology preserved visualization and computationally efficient algorithm. Besides, it also shows potential use in fully automated intelligent system where little or no human intervention is required. Future work may focus on inter-neurons distance preservation enhancement and probability density estimation for the projected map.

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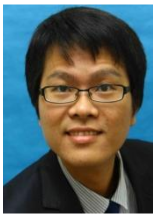

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