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Evaluating SOMs using Order Metrics

Arnulfo P. Azcarraga, PhD

PRIS Group, School of Computing, National University of Singapore
10 Kent Ridge Crescent, Singapore 119260
dcsapa@nus.edu.sg

ABSTRACT It has been shown that self-organized maps, when adequately trained with the set of integers 1 to 32, lay out real numbers in a 2D map in an ordering that is superior to any of the known 2D orderings, such as the Cantor-diagonal, Morton, Peano-Hilbert, raster-scan, row-prime, spiral, and random orderings. Two 2D order metrics (Average Direct Neighbor Distance and Average Unit Disorder) have been used to assess the quality of a map's 2D ordering. It is shown here that these same order metrics are useful in assessing the quality of the self-organization process itself. Based on these metrics, it can be determined whether the SOM has already adequately learned and whether the parameters used to train the SOM have been correctly specified. In applications like data analysis, where there is little clue as to the way the SOM is supposed to look like after training, it is important to be able to assess the quality of the self-organization process independent of the application.

1. Introduction

Kohonen's self-organizing maps (SOM) have been known to reflect topological relationships among input patterns and could thus graphically provide insights as to possible interesting relationships among the data items that make up the input environment [1,2]. Data visualization could be the basis for a subsequent data analysis, focused either only on specific variables and/or only on a subset of the unknown mass of data. In applications like data analysis, however, there is little clue as to how the SOM is supposed to look like after training. The user may have used the wrong training parameters, or the specific variant of the SOM may not be well suited to the specific data analysis application. In such cases, it is important to be able to assess the quality of the self-organization process independent of the application domain. In this paper, it is shown that this can be done using order metrics.

2. Quality of SOMs through Order Metrics

The concept of order of 2D maps refers to the degree by which spatially close map units are assigned values that are similar in the input environment. The order of 2D maps can be defined in exact and measurable terms using two order metrics: *Average*

Direct-Neighbor Distance (ADND) and *Average Unit Disorder* (AUD). A more complete description of ADND and AUD metrics appears in [1,2]. Some related information on 2D SOM order and neighborhood preservation can be found in [3,4].

Only the AUD metric will be described in this paper. Given a 2D map represented by a general graph whose nodes correspond to the map units arranged in a regular rectangular lattice. The weights $\mathbf{w}_{ij}$ of each node $\mathbf{u}_i$ are updated through self-organization. Each edge connecting nodes $\mathbf{u}_i$ and $\mathbf{u}_j$, has an associated label $\mathbf{l}_{ij}$. A given label $\mathbf{l}_{ij}$ is the average absolute difference between the weights of nodes $\mathbf{u}_i$ and $\mathbf{u}_j$. The AUD employs coefficients $\mathbf{c}_{ij}$ which are inversely proportional to the geometric distance between two nodes. Weighted labels $\mathbf{L}_{ij}$ between nodes that are more geometrically distant are assigned smaller coefficients, with $\mathbf{L}_{ij} = \mathbf{c}_{ij}\ \mathbf{l}_{ij}$, where $\mathbf{c}_{ij}$ is $1/\mathbf{d}_{ij}$ when i ≠ j, and $\mathbf{c}_{ij}$ is 0 when i = j. $\mathbf{d}_{ij}$ is the euclidean distance between $\mathbf{u}_i$ and $\mathbf{u}_j$. The disorder **UD**i of each unit is computed and the average for the entire map is the AUD. This way, the map's disorder distribution could be readily visualized. The AUD is computed as follows, where **N** is the number of units in the map :

$$UDi = \frac{\sum_{j=1,N} L_{ij}}{\sum_{j=1,N} c_{ij}} \qquad AUD = \frac{1}{N}\sum_{i=1,N} UDi \tag{1}$$

$$AUD = \frac{1}{N}\sum_{i=1,N} \frac{\sum_{j\neq i} l_{ij}/d_{ij}}{\sum_{j\neq i} \frac{1}{d_{ij}}} \tag{2}$$

Some ressemblance to the matching criterion in Sammon's non-linear projection algorithm [5,6,7,8] is noted. The so-called *measure of distortion* E is mimimum when the projection perfectly preserves the neighborhood relations among the patterns.

$$E = \frac{1}{\sum\sum_{i<j} d^*_{ij}} \sum\sum_{i<j} \left(\frac{(d^*_{ij} - d_{ij})^2}{d^*_{ij}} \right) \tag{3}$$

In the above formula, the distance between two patterns i and j is denoted by $\mathbf{d}^*_{ij}$ in the original feature space, and $\mathbf{d}_{ij}$ in the projected space. Note that in the AUD metric, $\mathbf{d}^*_{ij}$ is similar to $\mathbf{l}_{ij}$, since the unit's weights are known to converge towards the expected mean of the cluster of patterns to which each unit is sensitive, while $\mathbf{d}_{ij}$ is the same quantity in both the AUD metric and Sammon's measure of distortion.

In the earlier papers, it was shown that the ADND and the AUD can be used to assess the <u>outcome</u> (i.e. 2D ordering) of the self-organization process. In this paper, it is shown that these same order metrics are useful in assessing the quality of the self-organization process itself. Figure 1 shows the AUD values of the SOM when trained with the integer set {1,2, .. 32} for 100,000 training cycles (NB: to accentuate the

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shape of the AUD-curve, the graph only shows the first 30,000 cycles). The expected general shape for the AUD-curve is depicted in Figure 2. During the first learning cycles, when very few input patterns have so far been presented to the map, the units' weights are fairly alike, while some of the map units still contain remnants of the random initial values. The measure of disorder thus starts low and rises in value during the sensitization stage (i.e. the map becomes more and more disorderly) as the different map units are just being sensitized to the different input patterns. Once the sensitization stage is completed, the measure of disorder will have reached its peak and will begin to decrease in value. This marks the beginning of the global ordering stage. As the units' weights are updated, the ordering of the map improves, and this drives the values of the ADND and the AUD down. This trend continues until such a time when very little improvement can be done as far as the over-all ordering is concerned. This leads to the third stage, referred to as the fine-adjustment stage. At this stage, the changes in the units' weights are minute and so obviously, the measures of disorder stabilize.

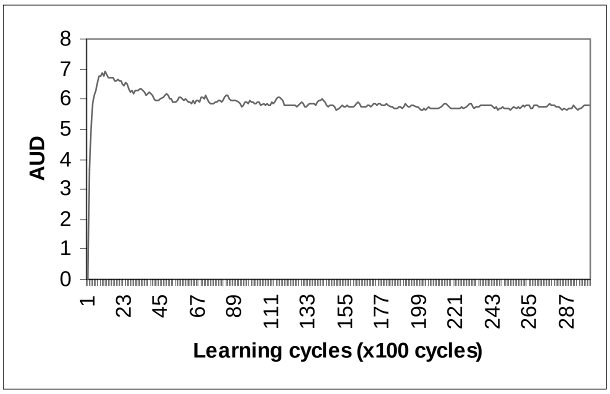

Figure 1 AUD-curve of the SOM when trained with the integer set {1,2, ..32}.

3. Order Metrics in Data Analysis

Numerous other experiments have been performed on SOMs, and the behavior of the order metrics *vis-à-vis* the ordering process has been quite consistent [2]. One experiment, which uses SOM to do data analysis on a set of real-world data, involves 423 student records containing the high school GPA, scores in 5 entrance examination sub-tests (English, Reading, Science, Mathematics, and Mental Ability), and grades in freshman subjects for the first and second terms. The trail of values for the AUD, plotted against the number of learning cycles, is shown in Figure 3. The sensitization stage happened during the first 1,000 cycles or so. Global ordering occurred from 1,000 to around 6,000 cycles, after which the fine-adjustment stage took over. With live data like in this case, the user may not have any concrete basis for knowing whether the self-organizing map has already fully "organized" itself. The use of order metrics is a good alternative – certainly a better alternative than requiring user intervention or specifying a maximum number of training cycles. Once the AUD does not change in value by more than some threshold, then training can stop.

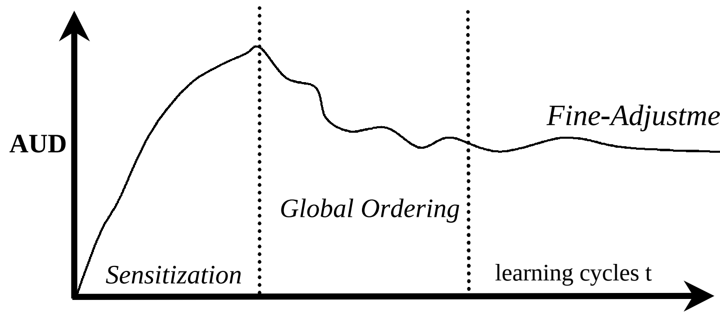

Figure 2 The expected shape of the AUD-curve

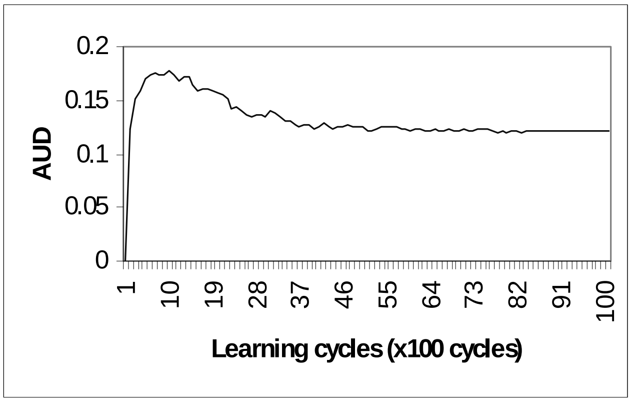

Figure 3 AUD curve reflects the quality of the self-organization process

More importantly, the user may not have any concrete basis for knowing whether self-organization ever took-place at all, i.e. whether the SOM algorithm was functioning correctly, or whether the parameters have been chosen properly. The usual approach is to try the algorithm and the set of parameters on toy problems, and once the algorithm seems to function properly, the same parameters are used for more important applications. Unfortunately, the conditions may have changed, and the same set of values for the parameters may no longer be appropriate. The user will have no way of knowing this. In such a case, the use of order metrics is a very attractive alternative.

Figure 4 shows the different AUD graphs for the same problem with the same map dimensions, same gain parameter, but different values for the ρ parameter (we used a variant of the SOM which integrates the decreasing neighborhood and gain size in a

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single learning rate function). The resultant maps for each of these runs are quite different given different values for ρ. In such a live case, there would have been no basis for distinguishing which SOM to use, as all of them seem plausible. However, note that in the figure, only those ρ values around 0.25 would result in the expected shape of the AUD-curve. Close inspection does confirm that the other SOMs either over-specialize or leave out large subsets of student records. The same type of experiment has been conducted on more controlled input sets, and the results all show that the AUD-curve must take the general shape described in Figure 2. Otherwise, the resultant maps do not conform to expected outcomes (which are known *a priori* for the more controlled input sets).

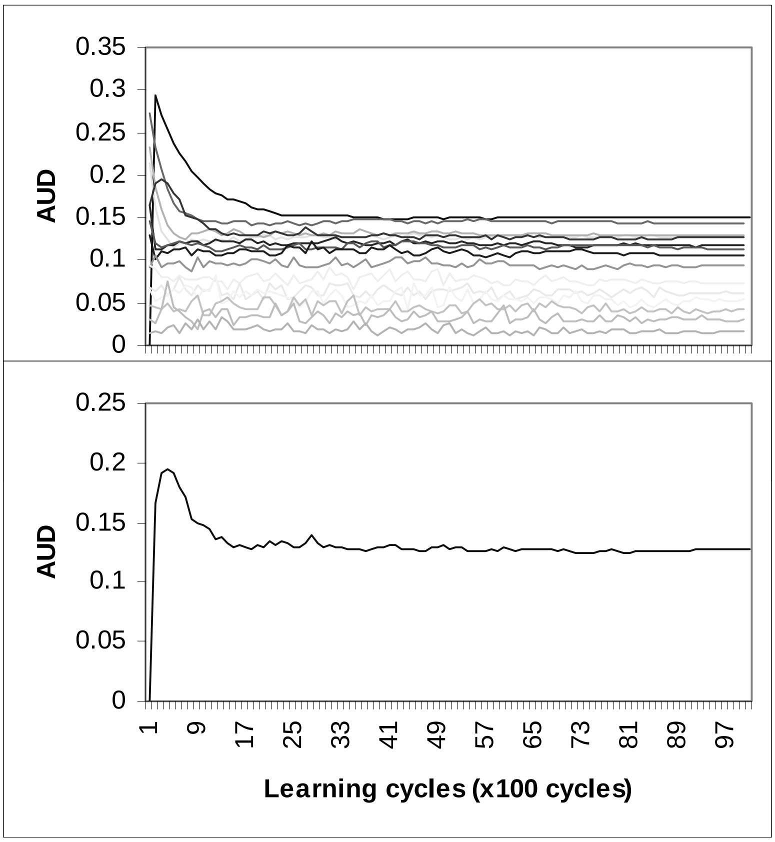

Figure 4 Different AUD graphs for different values for the ρ parameter. Only ρ values around 0.25 (lower graph) would result in proper self-organization.

The quality of the AUD-curve is visually matched against the “expected” general shape of the AUD curve. The evaluation as to when exactly can a given AUD-curve be considered acceptable is left to the user. More theoretical work is thus needed to fully characterize the relationship between the shape of the AUD curve and the quality of the self-organization process. Order metrics, we hope, will have the same role in the study of SOM covergence as does the “energy” in Hopfield Networks.

4. Conclusion

Designed to measure the degree by which spatially close map units are assigned values that are similar in the input space, the Average Unit Disorder (AUD) has been used to assess the quality of the 2D ordering produced by SOMs. This paper discusses how the same AUD metric can be used to gauge the quality of the self-organization process itself, i.e. to assess whether the user has used the correct training parameters, or whether the specific variant of the SOM is suited to the specific application. In applications like data analysis, there is little *a priori* information on the way the SOM is supposed to look like. In such cases, it is important to be able to assess the quality of the self-organization process independent of the application domain.

More theoretical work is needed to fully characterize the relationship between the shape of the AUD curve and the quality of the self-organization process. In the results presented in this paper, the quality of the AUD-curve is visually matched against the “expected” general shape of the AUD curve. This leaves plenty of room for subjective evaluation as to when exactly can a given AUD-curve be considered acceptable. All the experiments, however, seem to point clearly at the possible use of the shape of the AUD-curve as basis for assessing the quality of the self-organization process.

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