Organization Measures for Self-Organizing Maps

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Abstract

A quantification of the organization of SOM states is of interest from the viewpoint of theory as well as from that of application. The paper studies some properties of different organization measures for SOMs. Their behaviour is investigated and discussed for Maps with different topology trained with an equidistribution on the 2-dimensional unit square.

1 Introduction

When considering Neural Network models, often a distinction is made between supervised and unsupervised models. In the models of former class one often has some deviation of the present learning state of the Neural Network from the required one. In the models of latter class, however, usually the learning process is determined solely by the dynamics of the learning rule and there does not exist a canonical measure to determine the degree of training, or in the case of SOM, of their organization. Such a measure would be relevant not only for theoretical analysis of the organization process but also for practical purposes, as it could help to determine how well a trained SOM describes a given training set. In particular, such a measure would be interesting for higher dimensional data sets (e.g. speech data), where visualization is difficult or impossible.

The current paper concentrates on the study of the behaviour of several organization measures for the simple case of training using data from an equidistribution on the 2-dimensional unit square. The restriction to this simple case is warranted by the need to understand the behaviour of the SOM and the respective organization measures as fully as possible in a less complex context before using such measures with non-visualizable data sets where no intuitive inspection of the organization quality can take place.

What is an organization measure? We will not try to give a precise mathematical notion, as the required properties are currently difficult or impossible to realize with or to verify for the measures commonly regarded as organizational quantities. Instead, we wish to state informally the two properties relevant to our understanding of organization quantification as a starting point for the discussion. First, an organization measure should quantify the process of self-organization during the training, i.e. during the training the measure's average value should increase (or decrease) monotonously. Second, it should quantify the quality of the embedding of the *Kohonen graph* (see Sec. 2) into the input space (e.g. an untwisted "smooth"embedding of the square grid into the unit square should obtain a better value in this sense than the embedding of the linear grid into the same space). We will refer to these properties as to *Property 1* and *Property 2*.

The first of these intuitive requirements would be fulfilled by a Liapunov function for the deterministic dynamical system corresponding to the Kohonen Algorithm. Such one is given for the one-dimensional grid embedded into the one-dimensional interval by the number of inversions [9, 4]. There are different approaches for generalization of the inversion concept to the higher-dimensional case [3, 14], but to the author's knowledge no Liapunov function has been found yet for the general case. In particular, the existence of energy functions, i.e. functions fulfilling stronger criteria than a simple Liapunov function, has been ruled out for the one-dimensional case [6], a result which most probably holds also in the higher-dimensional case. Thus, currently, one can only hope to obtain some approximation to the ideal behaviour of a Liapunov function.

The second requirement is of even more interest, as it would provide ground to the assessment of SOM performance in non-visualizable cases. Here a precise specification of the required property is even more difficult and has been usually obtained by intuitive inspection of the embedding; quite recently a precise notion of well-organization of SOM states has been suggested [7]. It requires the set of (formal) *neurons* (or *units*) to be endowed not only with a metric, but also with some grid structure that allows the definition of notions of *dimension* and of a metric-compatible *basis*. The current paper however will only consider measures that can be defined for more general sets of *neurons*, where only a graph structure, the Kohonen graph, is imposed a priori. Furthermore the measures considered here will not characterize states as "organized" or "non-organized" in a binary yes/no sense, but will yield a different degree of organization for the respective embeddings.

We will study the following measures with respect to the above two requirements: the well-known mean quantization error μ_{Q} (it was felt that no distinction should be made between quantization and organization measures in the context of studying the measures w.r.t. Properties 1 and 2), the generalized inversion measure μ_{ZB} from [14], the topographic product μ_{BP} from [1], a measure μ_{DB} used for characterization of SOM states from [5], a measure μ_{H} developed in [2, 12] based on a Hebbian mechanism from [10] (that formed also independently the basis for the topographic function approach developed in [13]), and a hybrid measure μ_{QH} combining properties of this Hebbian measure with properties of the quantization error.

A discussion of the topographic function criterion from [13] will not be included in this paper, since an important feature of that approach is to calculate a complete function describing the SOM state embedding in different size scales, whereas our interests lie in the analysis of measures describing the SOM state using just one real-valued scalar. Also the recent measure from [8] will have to be left unconsidered.

2 Definitions and Conventions

We define the SOM as a map $\boldsymbol{w} : A \to V$ from a discrete finite set A of (formal) *neurons* to a convex subset V of $\mathbb{R}^d$, the *input space*, mapping each neuron j to its *weight* $\boldsymbol{w}_j$. On A the metric d_A is induced by the adjacency structure of an undirected graph without weights, the *Kohonen graph*, A being its vertex set, on V we choose the Euclidean metric. During the training we obtain a sequence $\left(\boldsymbol{w}(t)\right)_{t=1,2,\ldots}$ using the standard learning rule $\Delta\boldsymbol{w}_j(t) := \epsilon(t) \cdot h_t(\boldsymbol{i}^*_{\boldsymbol{w}(t)}(x(t)), j)(x(t) - \boldsymbol{w}_i(t))$ for all neurons j, $x(t)$ being the training input at time t, $\epsilon(t)$ the learning rate, h_t the activation profile and $\boldsymbol{i}^*_{\boldsymbol{w}(t)}(x(t))$ a neuron i minimizing the distance $d_V(x(t), \boldsymbol{w}_i(t))$ (in particular, $\boldsymbol{i}^*_{\boldsymbol{w}(t)}$ is a left-inverse map to $\boldsymbol{w}$). In the following we will write $\boldsymbol{i}^*$ instead of $\boldsymbol{i}^*_{\boldsymbol{w}(t)}$ for notational convenience.

3 Organization Measures

We give a short summary of the measures considered. The inversion measure μ_{ZB} from [14] is defined by $\mu_{\mathrm{ZB}} := \frac{1}{|\mathcal{C}_{\mathrm{K}}|\cdot(|A|-2)} \sum_{(j,k)\in\mathcal{C}_{\mathrm{K}}} D(j,k)$.

Here $\mathcal{C}_{\mathrm{K}}$ is the set of edges (j,k) of the Kohonen graph, $D(j,k)$ is the number of neurons $l \neq j,k$, whose receptive fields $\boldsymbol{i}^{*-1}(l)$ intersect of with the line between j and k. This sum is then normalized according to the number of possible connections and disturbances. A small value signifies good topology preservation, a high one distortions.

The topographic product μ_{BP} is defined as follows: Let $n_1^A(j), n_2^A(j), \ldots$ and $n_1^V(j), n_2^V(j), \ldots$ be the neurons from A sorted according to increasing A-distance $d_A(j, n_k^A(j))$ from j or V-distance of their weights $d_V(\boldsymbol{w}_j, \boldsymbol{w}_{n_k^V(j)})$, respectively. Then $Q_1(j,k) := d_V(\boldsymbol{w}_j, \boldsymbol{w}_{n_k^A(j)})/d_V(\boldsymbol{w}_j, \boldsymbol{w}_{n_k^V(j)})$ and $Q_2(j,k) := d_A(j, n_k^A(j))/d_A(j, n_k^V(j))$ measure the contribution to topology distortion by $\boldsymbol{w}$ or $\boldsymbol{i}^*$, resp., at the k-th distant neuron relative to j. Now with $P_3(j,k) := \left(\prod_{l=1}^k Q_1(j,l)Q_2(j,l)\right)^{1/2k}$ the final measure is given by a logarithmic average $\mu_{\mathrm{BP}} := \frac{1}{|A|\cdot(|A|-1)} \sum_{j=1}^{|A|} \sum_{k=1}^{|A|-1} \log\bigl(P_3(j,k)\bigr)$.

A value near 0 signifies good adaptation, negative values indicate folding of A into V (typically when "dimension" of A – considered as grid – is chosen too small), positive values indicate a topology mismatch in the other direction, i.e. a too large dimension of A.

The mean quantization error is calculated in our simulations choosing a large set $x_1 \dots x_q \in V$ of inputs by random according to the probability distribution on V. One obtains $\mu_{\mathrm{Q}} := \frac{1}{\mu_{\mathrm{Q}}^0}\sqrt{\frac{1}{q}\sum_{k=1}^{q} d_V\left(\boldsymbol{w}\left(\boldsymbol{i}^*(x_k)\right), x_k\right)^2}$, where μ_{Q}^0 is a normalization factor, derived from the (unreachable) theoretical lower bound for the quantization error obtained when assuming an equidistribution of signals around the weights in the closest possible way, i.e. on a disk (of course, in the 2-dimensional case one could have taken hexagons for the closest packing, but this method does not readily generalize to higher dimensions). The quantization error is then almost always greater than 1 (ignoring pathological simulation situations) and low quantization errors are desirable.

The measure introduced in [5] is given by $\mu_{\mathrm{DB}} = \sigma_w/\overline{w}$, where $\overline{w}$ is the average distance $d_V(\boldsymbol{w}_i, \boldsymbol{w}_j)$ between pairs of neurons i and j adjacent in the Kohonen graph and σ_w is the empirical standard deviation of these distances.

The Hebbian measure is based on the Delaunay triangulation of the set $\{\boldsymbol{w}_i | i \in A\}$ induced by the data distribution on V [10]. In practice one chooses according to this distribution a training set $x_1 \dots x_q \in V$. Whenever x_l lies in the 2nd order Voronoi cell V_{jk}^2 of $\boldsymbol{w}_j$ and $\boldsymbol{w}_k$ (i.e., whenever $\boldsymbol{w}_j$ and $\boldsymbol{w}_k$ are the weights nearest and second nearest to x_l), a Hebbian connection between j and k is created with strength $c_{jk} = 1$ if it did not exist before or, if it did, its strength is increased by one. Thus, one obtains a (second) graph with vertex set A whose edges have strengths c_{jk} estimating the value of $\int_{V_{jk}^2} p(x)dx$, p being the distribution density of data. This graph is compared to the original Kohonen graph determining d_A via $\mu_{\mathrm{H}} := 1 - \frac{\hat{c}\cdot|\mathcal{C}_{\mathrm{K}}\setminus\mathcal{C}_{\mathrm{H}}| + \sum_{(j,k)\in\mathcal{C}_{\mathrm{H}}\setminus\mathcal{C}_{\mathrm{K}}} c_{jk}}{\hat{c}\cdot|\mathcal{C}_{\mathrm{K}}| + \sum_{(j,k)\in\mathcal{C}_{\mathrm{H}}} c_{jk}}$.

$\mathcal{C}_{\mathrm{K}}$ as above denotes the edge set of the Kohonen graph and $\mathcal{C}_{\mathrm{H}}$ the edge set of the Hebb graph, $\hat{c} := \left(\sum_{(j,k)\in\mathcal{C}_{\mathrm{H}}} c_{jk}\right)/|\mathcal{C}_{\mathrm{H}}|$ being the average strength of the Hebb graph edges. There are slightly different possibilities for normalization, but typically the differences turn out to be small. The value of the deviation is subtracted from 1, thus μ_{H} gives values just below 1 for good matches, i.e. topology preservation and low values (but always $\mu_{\mathrm{H}} \geq 0$) for distorted embeddings. The Hebbian measure essentially determines the Kohonen edges that do not match Hebbian ones and vice versa. By weighting the edges, in particular the Hebbian, unsignificant edges are reduced in importance [2] and, in particular, the measure is rendered continuous at SOM states where a flip of Hebb edges takes place [12].

We will consider a further hybrid measure incorporating the Hebbian deviation measure and the quantization error; a short motivation for its use will be given during the discussion in Sec. 4. This hybrid measure has been defined by $\mu_{\mathrm{QH}} = \mu_{\mathrm{H}}/\mu_{\mathrm{Q}}^2$.

4 Simulations and Results

For the simulations the learning rate $\epsilon_t = 0.5/(1 + 0.004t)$ with activation profile $h_t(j,k) = 1$ for $d_A(j,k) \leq R(t)$ and $h_t(j,k) = 0$ for $d_A(j,k) > R(t)$ was used, setting the activation range $R(t) = 3$ for $t < 1000$, $R(t) = 2$ for $1000 \leq t < 2000$ and $R(t) = 1$ for $2000 \leq t$. Training runs included different network topologies, among them hexagonal and tree topology, but here we will restrict ourselves to the cases of a linear, a square and a $4 \times 4 \times 5$ ("cubic") grid as Kohonen graph. All SOMs consisted of 100 neurons. The input space V was 2-dimensional and the training signals were equidistributed.

Each training run has been extended to 300000 steps (note the logarithmic scale in Fig. 1) and has been performed independently 50 times for each topology. The measures depicted in Fig. 1 have been obtained by averaging over these 50 runs, the error bars indicate the empirical standard deviation thus calculated.

Property 1, i.e. monotonicity on average is fulfilled quite well for all considered measures except for μ_{BP} and μ_{DB} and even for these measures the region of non-monotonicity is limited to the

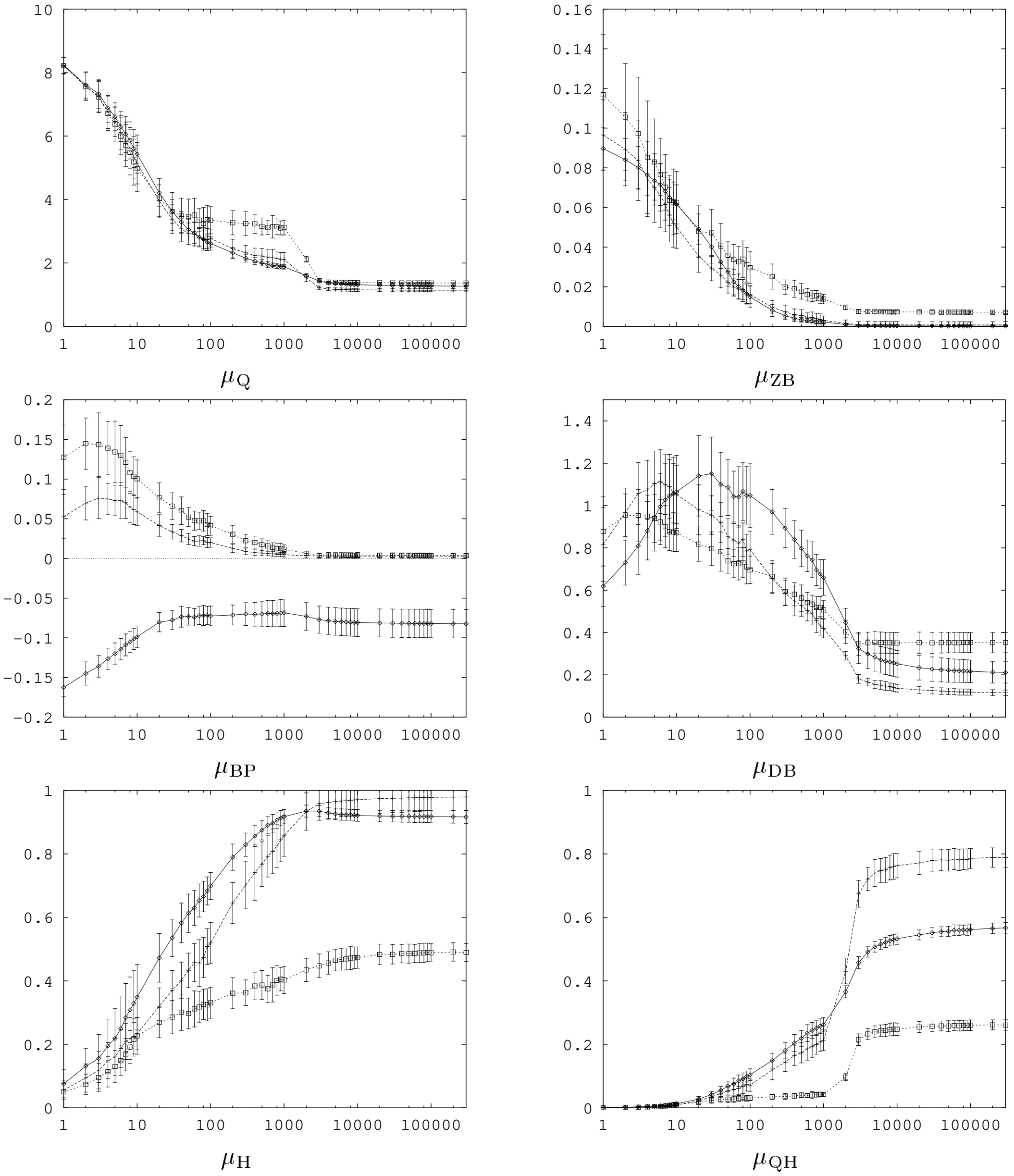

Figure 1: Learning curves for different measures, value vs. training step, solid line for linear, dashed for square and dotted for cubic nets.

initial training (i.e. the organization) phase; later in the training, during the fine-tuning phase, also these measures show monotonous behaviour. This shows that all measures considered are suitable candidates to be used as kind of “order parameters” for the quantification of the dynamics of the training process. Indeed, it is even possible to define a number of measures based on entropic considerations that all turn out to fulfil Property 1 for the examples considered [12], i.e. finding measures that comply with the requirements of Property 1 is an uncritical task.

This is different with Property 2. From Fig. 1 it can be seen that the range of values for μ_{Q} at the end of the runs (after long training) is very small compared to the value range attained during the first few thousand steps; therefore discrimination of the embedding quality of different SOMs via μ_{Q} would depend critically on the training phase and is in danger to be distorted by fluctuations when one does not extend the training to very long runs.

A similar effect can be seen with μ_{ZB}. Square and linear SOM attain values close to 0 within error range and cannot be distinguished. Even the "cubic" SOMs attain a very low value for μ_{ZB}. μ_{BP} shows a complementary problem. While the linear SOM is singled out very clearly (the negative values indicate a too low dimension for the square input space), μ_{BP} fails to distinguish between the square and the cubic SOM. Note that the discrepancy to the observations in [1] is due to the fact that via the Kohonen graph we implemented the $\|\,.\,\|_1$-metric on the set of neurons while in [1] the $\|\,.\,\|_2$-metric on A was used. Nevertheless, this indicates that the distinction capability of μ_{BP} for too high dimensions of A depends strongly on d_A and its reliability in this case therefore must be judged with care.

The next measure, μ_{DB} turns out to have a weaker distinction capability for the linear SOM than μ_{BP}, but a better one for the cubic SOM and is the first one in our discussion where at least the averages of all three topologies are clearly distinguishable. Nevertheless, the error bars of the linear SOM are still too large as to make it difficult to distinguish the quality of the linear topology from the square one in a single run. Note that for the plots of the values of μ_{DB} (and also for μ_{QH}) we did not include those seven of the fifty training runs for the square topologies where the SOMs showed twists and folds; the reason was that these measures were particularly sensitive to those twisted embeddings and thus produced two clusters of values, a small cluster of worse values for the embeddings with topological defects and a larger one for those without. In particular w.r.t. Property 2 this capability of μ_{DB} and μ_{QH} is quite desirable, as one would expect an organization measure to detect embedding defects. On the other hand, the runs for μ_{Q}, μ_{ZB} and μ_{BP} show the latter to be rather insensitive to such defects.

Including the runs with defective embeddings for the average and error calculation of μ_{DB} and μ_{QH} would distort the picture, since the significantly larger error bars and worse measure values then obtained are only due to their capability to identify the existence of two clearly different embedding classes. Such a distinct classification of correct and defective embeddings does not make sense for linear and cubic SOMs and was not observed in the distribution of measure values.

μ_{H}, as preliminary stage to μ_{QH}, displays a very clear distinction of the cubic SOM, its distinction capability between linear and square grids is however limited, even though it is better than μ_{Q} and μ_{ZB} (note that for demonstration purposes here we included the runs with defective square SOMs, therefore the large error bars for this case, since μ_{H} is sensitive to defects). The reason for the small difference between the value for the square and the linear SOM is discussed in [11, 12].

The last measure considered here is μ_{QH}. The reason for introducing this measure have been investigations using Genetic Algorithms (GAs) for the optimization of SOM topologies [11].

First μ_{Q} and μ_{H} were used as optimization criteria for the GAs. It was then found that both measures produced topologies that displayed – in a way – "orthogonal" properties. However, either did not suffice to obtain what one would intuitively call a topologically correct embedding. This and related observations led to the introduction of the hybrid measure μ_{QH} as optimization criterion, which proved to consistently generate SOMs of the desired structure during the GA. Fig. 1 shows that μ_{QH} is able to discriminate the square SOM very clearly from the other SOMs. Above GA results indicate that the capability of μ_{QH} to discriminate topological correct embeddings from defective ones is significant, since in the GAs the search space for topologies included a large class of different Kohonen graphs and not only selected examples.

5 Summary and Outlook

Finding good organization measures describing the embedding quality of SOM states is relevant for theory and applications, namely for studying their dynamics and for assessing the quality with which they model a given data space. Due to a lack of a canonical quantity a multitude of organization measures have been defined. We studied several of those measures that were motivated by different theoretical or practical considerations. While almost all measures investigated approximately fulfil the monotonicity condition, even in the simple and clear-cut cases considered here, most measures display considerable limitations w.r.t. the identification of inadequate embeddings:

the main problem is the identification of both, the linear and the cubic SOM as inadequate. In this respect μ_{DB}, and, even more pronounced and moreover backed up by investigations using Genetic Algorithms, μ_{QH} presented here, perform best.

On the other hand, the results show that in the current state of research one must proceed with great care when applying some organization measure to new situations with no a priori knowledge of the structure of the training data. Therefore, future work will have to further concentrate on a detailed analysis of the behaviour of the measures mentioned in well-known and controlled domains for the case of higher dimensional data and for not equidistributed data. An incorporation of the measure from [8] and of the non-scalar measure from [13] in the investigations is also envisaged in the future.

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