Measures for the Organization of Self-Organizing Maps

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Abstract. The “self-organizing” dynamics of Self-Organizing Maps (SOMs) is a prominent property of the model that is intuitively very accessible. Nevertheless, a rigorous definition of a measure for the state of organization of a SOM that is also natural, captures the intuitive properties of organization and proves to be useful in practice, is quite difficult to formulate. The goal of the paper is to give an overview over the relevant problems in and different approaches towards the development of organization measures for SOMs.

1 Introduction

1.1 Self-Organization

The first use of the notion of “self-organization” can be traced back to 1947 (Ashby 1947; Shalizi 1996). Yet, through the last half-century, a satisfactory universal definition of self-organization has not been found. Instead, the degree of self-organization has always been measured with measures constructed *ad hoc* for the system at hand, requiring some interpretation of the system induced by an observer.

Kohonen Maps represent the phenomenon of self-organization in such a paradigmatic way that they are often simply referred as *Self-Organizing Maps* (SOMs), as in the title of this review. The whole spectrum of questions associated with the phenomenon of self-organization emerges in conjunction with the study of SOMs. The topic of the present review bears close relations to this fundamental question. Because of the limitation of this review's scope, this question will not be studied in its own right, but its connection to the present discussions should always be borne in mind.

1.2 Supervised and Unsupervised Learning

An important distinction that is made in the study of neural networks is determined by the learning rule which is applied to the network under consideration. Learning rules are divided into the main classes of *supervised* and *unsupervised* rules as well as into some smaller classes which cannot be associated with the former classes in a definite way and which will not be considered further.

In the supervised case, the teacher provides a set of training examples, each of which consists of input data and corresponding target output data.

The usual application of neural nets is then to model an input-output relation implied by this data set. The learning rule is expected to achieve a "suitable" correspondence between the target and the actual output values by adapting the structure and weights of the network. The suitability is measured by an explicit deviation function; e.g., in the case of backpropagation networks, by the squared error $1/2 \sum_\mu \|\mathbf{y}^{(\mu)} - \psi(\mathbf{x}^{(\mu)})\|^2$, where $(\mathbf{x}^{(\mu)}, \mathbf{y}^{(\mu)})$, are the input-output pairs of the training data and $\psi(\mathbf{x}^{(\mu)})$ is the real output of the network when the input $\mathbf{x}^{(\mu)}$ is applied.

In the unsupervised case, however, no target output and no explicit deviation from a learning target is specified. In the case of Kohonen's SOM, however, the dynamics of the system is given *a priori* by the learning rule and not derived from some explicit measure of deviation from a target state. Nevertheless the Kohonen learning algorithm causes a process to take place which human intuition is prone to describe as "self-organizing". The "organization" of the system can be intuitively detected by visual inspection of the graphical representation of SOMs during training. But "intuitive detection" and mathematical quantification are different things. This is in contrast to supervised learning methods with a canonical organization measure. Such a measure would determine how well data are being described by the neural network. For a self-organizing network such a measure would provide some a priori characterization of intrinsic organization.

In the presentation, no explicit distinction will be made between different types of notions, like organization measures, quantization measures, notions or measures of topology preservation. Instead, throughout the paper the term *organization measure* will be used for functions that assign real values to a SOM in a given state if it fulfills certain conditions (Sec. 2.4).

1.3 On this Paper

Before embarking on details of the different models, some remarks are in place to make clear how this paper should be used. The paper provides an introduction, overview and categorization of a large selection of different approaches to quantify organization in SOMs and topographic mapping models related to it. The selection of available approaches is vast and cannot be comprehensively treated, so this review will concentrate on most important and influential approaches and give pointers for further information. The idea is to provide the reader with an overview of the most relevant aspects of structure, philosophy and properties of currently existing approaches and with pointers for more extensive studies.

2 General Aspects and Definitions

In general, we will assume two spaces, an *input space* V and an *output space* A, to which signals from V are mapped. The input space considered will often be continuous (typically the $\mathbb{R}^d$), the output space will often be discrete, but sometimes we will consider other types of output spaces, too.

2.1 A Typology of Organization Measures

Several aspects are important to distinguish the different approaches to measure organization. We will discuss them in the following.

1st-order vs. 2nd-order measures We do not only consider "pure" organization measures that quantify the organizational structure of the mappings, but also include measures of distortion or quantization and information transmission (entropy). The reason is that the latter measures can be considered *1st-order measures*, whereas the former are *2nd-order measures*. If we speak of 1st-order measures, we intend to say that the measure value is obtained by combination of values (e.g. activation frequency or intensity) obtained for individual neurons, whereas in 2nd-order the final value of the measure results from a combination of values (e.g. similarity or distance) obtained for pairs of neurons into a single number.

Data-orientation The approaches to measure organization can be classified according to whether they include the structure of the data to map in their quantification or not. With data-oriented measures, Structurally equivalent mappings can thus obtain completely different measure values for the same type of measure, depending on the structure of the data.

Dynamics and structure The construction of many measures is oriented at quantifying the quality of typically the final stage of a mapping. The quantification of the dynamic development of the mapping is usually considered in a separate context since in general. Typical representants for measures of the dynamics are Liapunov functions. This class can sometimes be specialized to consider energy functions, if they exist. There exist mapping scenarios (see (Graepel et al. 1998) and also Sec. 3.3), for which an energy function can be formulated. Note that it is not obvious what a Liapunov function has to do with what we consider a good organization. Nevertheless it is important for mathematical analysis of the training process.

Predicates, measures and order parameters There are several notions of topology preservation that just distinguish the cases of a mapping being ordered or not. However, this characterization has a different quality than measures that attribute a numerical value to the disordered case. The first case can be regarded as a logical predicate that defines the notion of a mapping being ordered (or disordered) in a strict mathematical sense. When, say, the ordering predicate is not fulfilled, then the *degree* of disorder, i.e.

the deviation from the ordered case can now further be quantified. For the quantification of the deviation there exists a high degree of arbitrariness.

An organization measure could be devised in such a way that it attains some extreme (either minimum or maximum) value for the ordered case and deviates from that value the “farther” in the disordered regime the mapping is. We find types of this kind of measures in (Villmann et al. 1997; Goodhill et al. 1995).

The philosophy is similar to that of *order parameters* known for thermodynamics (Reichl 1980). Order parameters are used in physics to distinguish different types of equilibrium states in physical systems. Usually, they are chosen such that their value vanishes in states with a higher distributional symmetry and deviates from 0 when the symmetry of the state distribution is broken. The order parameter view has been directly used for the study of SOMs and related models (Ritter and Schulten 1989; Der and Herrmann 1993; Graepel et al. 1997). A study that reverses that direction and uses an independently constructed organization measure (Zrehen and Blayo 1992) as a kind of order parameter is (Spitzner and Polani 1998).

Topology and geometry Mapping organization is often seen as equivalent to topology preservation. In the strictest sense, most measures are not measuring topology preservation. Instead, they use a mixture of topological, similarity, metrical, or even further geometrical properties of the spaces mapped. The measures may be incorporating similarity or metric values themselves or just their relative ordering.

We give a short classification over some of the approaches.

“Pure” topology measures Only very few measures for organization have been formulated in notions of “pure” topology. One of the problems in finding such a formulation that one of the spaces involved in a SOM mapping is usually discrete. For these spaces, the canonical topology is the discrete topology. This is a very uninteresting case since it essentially implies a complete lack of structure..

One approach to explicitly solve the problem has been brought forward in (Villmann et al. 1997) by using a collection of “marked” discrete spaces on which a topology is defined w.r.t. to the respective marked element. This approach requires an extension of the regular notion of topology on the discrete space. In addition, the topological structures considered by Villmann et al. are induced by metric structures.

Driven from considerations of the maximization of information transmission by the mappings, equiprobable mapping methods have been investigated (Hulle 1997; Van Hulle 1997; Hulle 2000). In the present review, we wish to point out that the structure introduced in that papers on the discrete space can be interpreted as a *complex*, a structure known from algebraic topology (Henle 1979). A complex can be seen as a generalization of the notion of a graph. However, no invocation of metric structures is required for its definition, thus the method and the measures derived from it can be regarded as a truly pure topological notions.

Similarity and metrics In the spaces, the pairs of elements have to be compared for the mapping organization to be quantified. This can happen on the graph level by determining whether the elements of the space are adjacent. A second, more general way of doing it is to define a measure on the space that determines how similar the elements of the space are. a similarity measure needs not to have a metric or geometrical interpretation as opposed to a metric which has to fulfil the triangle inequality. The triangle inequality of a metric, on the other hand, can be interpreted as a kind of geometrical generalization of the transitivity property of a linear ordering relation.

It is therefore quite natural to include graph-based spaces at this point. A graph can both be interpreted as a topological and as a metrical structure. However, it is not possible to fully exploit the graph structure as a purely topological construct in the case of more than $k = 1$ dimensions and one has to resort to structures like *topological complexes* (Sec. 3.7). However, there is always the possibility to exploit the graph as a metric (and thus, e.g. via some neighborhood function also as similarity quantity). This makes the graph structure to a very natural model for the output space V. Indeed, in many mapping scenarios, output spaces are modeled as graphs.

Geometry Further geometrical properties are used only by very few models to quantify organization. Alder et al. (1991) present an approach that assumes a rectangular grid as output space and is related to curvature measures of Riemannian spaces.

2.2 Definitions

We have seen in Sec. 2.1 that for the output space graph structures prove to be the most versatile models. Therefore, in the definition of the basic SOM model the output space will be based on a graph.

Definition 1 (Self-Organizing Map). Define the *state of a SOM* as a map $\mathbf{w} : A \to V$ 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* $\mathbf{w}_j$. We will often simply say SOM instead of SOM state.

Let $\mathcal{C}_\mathrm{K} \subseteq A \times A$ be the adjacency structure of an undirected graph without weights with the set A of neurons as vertex set. This graph will be called the *Kohonen graph.*

The Kohonen graph induces a metric d_A on A, by defining $d_A(i, j)$ as the minimum distance between two neurons $i, j \in A$, where $d_A(i, j) = 1$ for two adjacent neurons. Unless stated otherwise, on V the Euclidean metric is used as d_V.

Given an initial SOM state $\mathbf{w}(0)$, a SOM training sequence $\big(\mathbf{w}(t)\big)_{t=1,2,\ldots}$ is defined by the applying the Kohonen learning rule

$$\Delta\mathbf{w}_j(t) := \epsilon(t)\cdot h_t\Big(\mathbf{i}^*_{\mathbf{w}(t)}\big(x(t)\big), j\Big)\big(x(t) - \mathbf{w}_i(t)\big) \ , \tag{1}$$

to all neurons j with $\Delta\mathbf{w}_j(t) = \mathbf{w}_j(t+1) - \mathbf{w}_j(t)$. Here $x(t)$ is the training input at time t, $\epsilon(t)$ the learning rate, h_t the activation profile and $\mathbf{i}^*_{\mathbf{w}(t)}$ a function where $\mathbf{i}^*_{\mathbf{w}(t)}(x(t))$ is a neuron i minimizing the distance $d_V(x(t), \mathbf{w}_i(t))$. In the following we will write $\mathbf{i}^*$ instead of $\mathbf{i}^*_{\mathbf{w}(t)}$ for notational convenience.

V is called *input space*. $\mathbf{i}^*$ is the *quantization function*. For $x \in V$, we say that input signal x *activates* the neuron $\mathbf{i}^*(x)$. For a given neuron i, the set $V_i := \mathbf{i}^{*-1}(i)$ of inputs from V that activate this neuron is called its *receptive field*. Its closure, $\overline{V_i}$, is called the *Voronoi cell* of i w.r.t. the set of points $\{\mathbf{w}_k \mid k \in A\}$ if d_V is Euclidean. In that case, for a given SOM state $\mathbf{w}$, the receptive field of a neuron i is uniquely defined on its interior except for a Lebesgue null set[1].

The quantization function $\mathbf{i}^*$ can be regarded as a lossy compression for signals from V into an event represented by a neuron $i \in A$. The inverse direction is information-conserving, as $\mathbf{i}^*_{\mathbf{w}}$ is a left-inverse map to $\mathbf{w}$.

2.3 Metrics and Topology

The restriction to graph-induced metrics or *graph metrics* on A nevertheless enables the realization of important metric structures on standard configurations like an n-dimensional grid. Fig. 1 shows the realization of two particular metrics on a 2-dimensional grid of neurons. The $\|.\|_1$- and $\|.\|_\infty$-metric can be realized, however not the (Euclidean) $\|.\|_2$-metric.

The intuitive notion of the output spaces being e.g. one-, two- or higher-dimensional grids (particularly rectangular ones) is widely used in the literature (e.g. (Ritter et al. 1994)). Since our investigations will also consider more general metric structures of A, it is sometimes advantageous to cast this somehow vague notion into a more precise definition (Polani 1995, 1996). Here, when talking about the dimension of a grid, we will appeal to the reader's intuition.

2.4 Requirements for an Organization Measure

Due to the lack of a canonical notion or measure of SOM organization, there is a considerable amount of arbitrariness, i.e. of "degrees of freedom", for its choice. It will be therefore necessary to clarify the requirements that should qualify a notion of SOM organization. Let $\mathcal{W}_{A,V} \equiv \mathcal{W}$ be the set of maps

[1] If the metrics is non-Euclidean, "pathological" cases can occur where the sets of ambiguous inputs need not be Lebesgue null sets (Polani 1996).

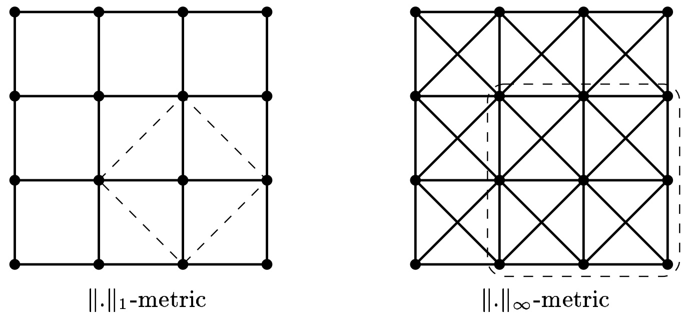

Fig. 1. Realization of different 2-dimensional metric structures by Kohonen graphs. The dashed regions indicate the "unit circles" of the corresponding metrics.

with output space A and input space V. We wish to state informally two properties which would qualify a function

$$\mu : \mathcal{W}_{A,V} \to \mathbb{R}$$

to be called an organization measure:

1. It should quantify the process of self-organization during training, i.e. its value should increase (or decrease) monotonously on average.
2. It should measure the quality of the embedding of A into the data manifold, i.e. the embedding shown in Fig. 2(a) should obtain a "better" value than, say, the embedding shown in Fig. 2(b).

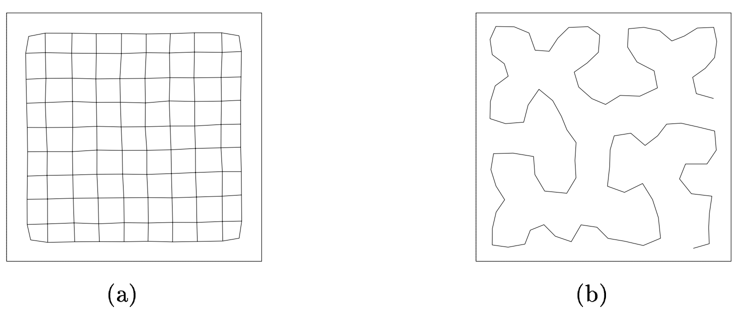

Fig. 2. Kohonen maps with different embedding quality

The first condition is of interest for mathematical analysis and for the understanding of the organization process. The second one is important for applications which have to estimate the quality of the description of a high-dimensional data manifold by the SOM.

However, an organization measure need not fulfil both properties. Indeed, it is not even clear that a measure μ fulfilling but the first condition could be found. The second property is not a hard constraint as the first, as different measures will most probably yield different estimations for ambiguous cases of embeddings (e.g. when the data manifold consists of several components of different dimension).

Since the first property can be cast into precise form in a fairly straightforward way, one would choose as first candidates for a discussion as organization measures such μ having this property. We can demand a weaker and a stronger version of property 1. The weaker version would only require μ to be a Liapunov-function, i.e. that the μ-measure would decrease on average during the training, or formally

$$E\Big(\mu(\mathbf{w}(t+1))\Big) \leq \mu(\mathbf{w}(t))$$

for all $\mathbf{w}(t) \in \mathcal{W}$, $t \in \mathbb{N}$, E denoting the average over a random training signal.

Organization measures can express a deviation, i.e. their value drops when organization becomes better during training or their value may grow during the self-organization process. Yet other sorts of information can be obtained by an organization measure (see Sec. 3.6).

3 Measures of Organization

3.1 Inversion measures

For the case of a one-dimensional net with $A = \{1 \dots n\}$ and V a subinterval of $\mathbb{R}$ a Liapunov-function can be given. Following (Cottrell and Fort 1987; Cottrell et al. 1994) and (Kohonen 1989) an organization measure μ_1 can be chosen as the number of inversions, i.e. as

$$\mu_{\mathrm{Inv}}(\mathbf{w}) = \left| \Big\{ i \in \{2 \dots n-1\} \;\Big|\; \mathrm{sgn}(\mathbf{w}_{i+1} - \mathbf{w}_i) \neq \mathrm{sgn}(\mathbf{w}_i - \mathbf{w}_{i-1}) \Big\} \right| \; .$$

In other words, μ_{Inv} counts the times change of directions takes place while i runs from 1 to n. The convergence theorems in above references guarantee that μ_{Inv} thus defined possesses property 1.

As the restriction to dimension 1 is not sufficient for applications, a generalization of this measure to a measure μ_{ZB} on $\mathcal{W}_{A,V}$ for open convex subsets $V \subseteq \mathbb{R}^n$, $n > 1$ has been formulated in (Zrehen and Blayo 1992). It is given by

$$\mu_{\mathrm{ZB}}(\mathbf{w}) = \frac{1}{|\mathcal{C}_K| \cdot (N-2)} \sum_{(i,j) \in \mathcal{C}_{\mathrm{K}}} D(i,j) \; ,$$

where $\mathcal{C}_{\mathrm{K}}$ is the set of adjacency pairs $(i,j) \in A \times A$ in the Kohonen graph and $D(i,j)$ is the number of receptive fields of neurons $k \neq i,j$ intersecting with the line from $\mathbf{w}_i$ to $\mathbf{w}_j$. The factor $1/|\mathcal{C}_\mathrm{K}| \cdot (N-2)$ normalizes the measure according to the number of possible connections and disturbances.

However, there is no monotonicity theorem guaranteeing a decrease (on average) for μ_ZB. Therefore it is not clear, whether it can be considered as a Liapunov function for the SOM.

3.2 Entropy

In (Linsker 1988) the information transmission from input to output has been studied for a specialized class of feed-forward neural networks. The investigations showed that under certain conditions the learning process of those networks can be observed to express a maximization of information preservation in the data transmission from the input to the output neurons. This suggests using an information-theoretic principle for the design of networks, *Linsker's infomax principle* and its variants (Haykin 1999). Neural network architectures are not necessarily explicitly designed to obey the infomax principle, but having a look at their information preservation capabilities may promise to yield a better understanding of their information processing properties.

The activation process of a SOM can be considered as a transmission mechanism for information which transfers signals hitting the input space V into signals in the output space A (Hulle 2000). For this information transfer process different kinds of entropies can be calculated; here we concentrate on the *neuron activation entropy* or simply *neuron entropy.*

The neuron entropy attains its maximum when probability of activation is the same for all neurons, i.e. when when all receptive fields have the same probability to be hit under the distribution P. Maximal entropy signifies that the quantization of the input space takes place in a best possible way; of course only the quantization class is then specified as precise as possible with the neurons available and not the position of the incoming signal. The simple neuron entropy does not know anything about the geometrical properties of the embedding of $\mathbf{w}$ in the input space. What neuron entropy can tell us is of purely information-theoretical nature. As long as the receptive fields have the same probability to be activated it does not play a role whether they might be long and narrow, thus leading to a high quantization error μ_Q or close to ideal sphere packing for equidistributed input signals.

Let an input signal distribution be given. If the probability that a neuron i is activated by an input signal is given by p_i, the neuron activation entropy is given by

$$-\sum_{i \in A} p_i \log p_i \ ,$$

The entropy can be seen as that amount of Shannon information that is conveyed by the mapping. Here the activations of the individual neurons are elementary. In that view, the individual activations cannot be compared to

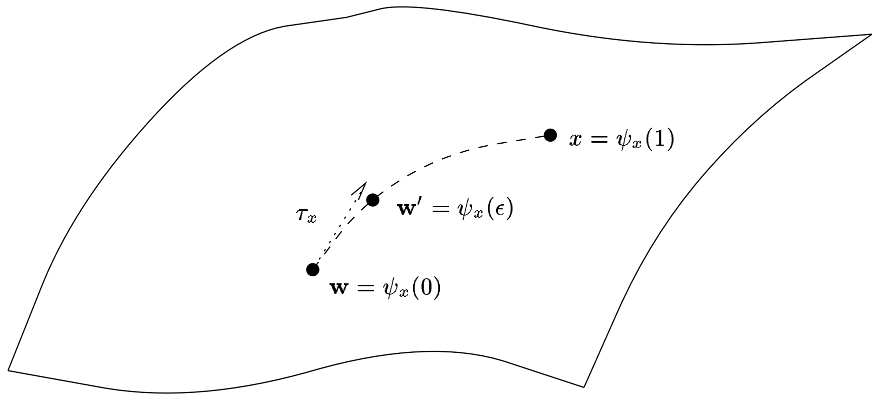

Fig. 3. $\psi_x(\epsilon)$

each other since it does not assume any semantics structure on the set of transmitted events, and thus also no similarity. In particular, the entropy needs not at all be related to topology preservation.

3.3 Energy Function Measures

It would be desirable to have an organization measure with stronger properties than are required for a Liapunov-function (Wiskott and Sejnowski 1997; Heskes 1999). Such a measure could be obtained by using an *energy function* for the training rule.

Definition 2 (Energy Function). Let $\big(T(\epsilon)\big)_{\epsilon\in[0,1]}$ be collection of learning rules with

$$\mathbf{w}_i(t+1) = [T(\epsilon)(x, \mathbf{w})]_i \ ,$$

for $i \in A$ and where ϵ is the learning rate. Assuming fixed $x \in V$ and $\mathbf{w} \in \mathcal{W}$, then $\psi_x(\epsilon) := T(\epsilon)(x, \mathbf{w})$ is a differentiable curve in ϵ with $\psi_x(0) = \mathbf{w}$, which allows us to define

$$\tau_x(\mathbf{w}) = \frac{d\psi_x}{d\epsilon}(0) \ ,$$

which is a vector in the tangent space $T_{\mathbf{w}}\mathcal{W}$ of $\mathcal{W}$ in $\mathbf{w}$ (see Fig. 3 and also (Abraham et al. 1983; Forster 1984)).

Since τ_x is defined for every $\mathbf{w} \in \mathcal{W}$, τ_x defines a vector field on $\mathcal{W}$. A differentiable function $U_x : \mathcal{W} \to \mathbb{R}$ is called *energy* or *potential* function for the learning rule T if

$$dU_x = \tau_x^\flat \ ,$$

where $\tau_x^\flat$ denotes the adjoint 1-form to the vector field τ_x via the canonical metric[2] on $\mathcal{W}$ (notation from (Abraham et al. 1983)). If x is a random variable then

$$\tau := \mathbf{E}(\tau_x)$$

defines a vector field on $\mathcal{W}$ ($\mathbf{E}$ denoting the expectation value w.r.t. the distribution of x). In analogy to above a function $U : \mathcal{W} \to \mathbb{R}$ is called *energy* function for τ if $dU = \tau^\flat$.

In certain cases it is possible to specify an energy function explicitly.

Energy Function for Training Signal with Discrete Support. If the training signal is concentrated on a set $\{\hat{x}_1, \ldots, \hat{x}_q\}$ which are assumed to have probabilities $p_1, \ldots, p_q$, the function

$$U(\mathbf{w}) = \frac{1}{2} \sum_{i,j} \left(h(i,j) \sum_{\hat{x}_k \in V_j(\mathbf{w})} p_k d_V(\hat{x}_k, \mathbf{w}_i)^2 \right) \tag{2}$$

is an energy function for the learning rule (Ritter et al. 1994).

Energy Function for 0-Neighbour Case (Quantization Error) For a SOM with $A = \{1, \ldots, n\}$, $h(i,j) = \delta_{ij}$ (δ_{ij} denoting the Kronecker delta) and a training signal with probability density p a potential function is given by

$$U(\mathbf{w}) = \sum_{i=1}^{n} \int_{V_i(\mathbf{w})} d_V(\mathbf{w}_i, x)^2 \, p(x) dx \text{ (Cottrell et al. 1994).} \tag{3}$$

This is identical to the squared mean quantization error.

The mean quantization error does not contain any information about topology. However, a connection between the quantization error and the organization of the SOM can be made. Luttrell (1989) shows that by minimizing the quantization error and assuming a suitable error model on the output space, one arrives at a learning rule similar to the SOM. Furthermore, (Ritter et al. 1994) show that a neighborhood improves convergence. This also is observed for other topographic mapping models (Hulle 2000). In (Polani 1996), it is shown that to enhance a fast improvement of the quantization error, a Genetic Algorithm optimization creates a neighborhood, but this neighborhood needs not be topology preserving (Polani and Uthmann 1992, 1993).

[2] Assuming $V \subseteq \mathbb{R}^d$, $\mathcal{W}$ can be identified with a subset of $\mathbb{R}^{d \cdot N}$, inheriting the corresponding metric.

Nonexistence of Energy Function for the Continuous Case However, for a case as simple as the SOM with grid dimension 1, the question whether there exists a potential function for more general h or for a continuous distribution of x has been answered negatively. Indeed, by use of an elegant argument, even a stronger result is shown in (Erwin et al. 1992a). As it gives insight into the complex configurations that can arise in the general case, we give a reformulation of the argument in the language of differential forms subsequently yielding a geometric interpretation.

The analysis in (Erwin et al. 1992a) is focused on SOMs with one-dimensional grid topology, with $A = \{1, \ldots, n\}$ and $V = [0, 1]$. As training input an i.i.d. sequence of random variables $(x_t)_{t\in\mathbb{N}}$ is considered, distributed according to the uniform distribution on $[0, 1]$. Analysis of the vector field τ discussed above is restricted to the subset $\mathcal{W}' \subseteq \mathcal{W}$ with

$$\mathcal{W}' = \{\mathbf{w} \in \mathcal{W} | \mathbf{w}_i \neq \mathbf{w}_j \text{ for } i \neq j\} ,$$

the complement $\mathcal{W} \setminus \mathcal{W}'$ of which is a Lebesgue-null set. To simplify calculation, τ is considered only on the subset

$$\mathcal{W}'' = \{\mathbf{w} \in \mathcal{W} | \mathbf{w}_i < \mathbf{w}_j \text{ for } i < j\}$$

and extended to $\mathcal{W}'$ by application of permutations of A, making use of symmetry properties of $\mathcal{W}'$.

The existence of a function U with $dU = \tau^\flat$ requires $d\tau^\flat$ to vanish, which does not happen in general. Indeed, even the weaker condition

$$d\tau^\flat \wedge \tau^\flat = 0 \qquad (4)$$

($\wedge$ denoting the wedge product of differential forms) is not fulfilled in general, as demonstrated in (Erwin et al. 1992a). By the Frobenius theorem (Abraham et al. 1983), this implies that $\tau^\flat$ is not integrable or, equivalently, $\tau^\flat$ cannot be represented as $g\,dU$ with suitable functions $g, U : \mathcal{W} \to \mathbb{R}$. Integrability of the form $\tau^\flat$ would have an immediate geometrical interpretation. It would mean that locally there would exist a system of submanifolds of $\mathcal{W}'$, the tangent bundles of which would be annihilated by $\tau^\flat$. In other words, if M were such a manifold, $\tau^\flat(v)$ would vanish for a vector v from a tangent space $T_{\mathbf{w}}M$, i.e. $T_{\mathbf{w}}M$ is perpendicular to τ (Fig. 4). The importance of the non-integrability of $\tau^\flat$ arises from the fact that this implies the nonexistence of local "equipotential" submanifolds M (whose tangent spaces $T_{\mathbf{w}}M$ would be perpendicular to τ at every $\mathbf{w} \in M$).

Modified SOM Algorithms and Energy Functions There exist further modifications of the SOM algorithm and similar models that allow the formulation of an exact energy function for the learning algorithm, e.g. (Wiskott and Sejnowski 1997; Graepel et al. 1997, 1998; Heskes 1999; Hulle 2000).

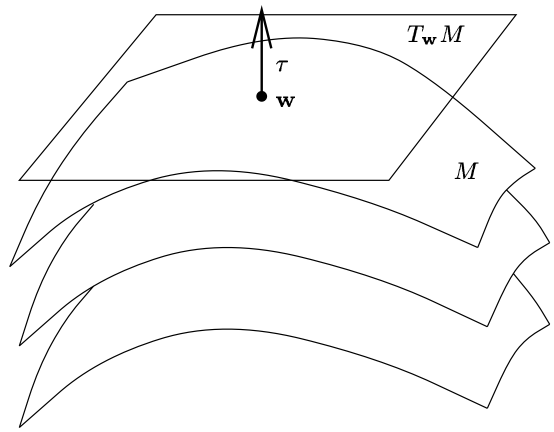

Fig. 4. Geometrical interpretation of integrability at point with nonvanishing τ

These cannot be discussed here in detail and we refer the readers to the original works.

The question may now be why one would bother to study the original SOM algorithm which poses so much resistance to conventional mathematical analysis. A reason to do so is that the simplicity of the SOM learning rule on the one hand and the complexity of its mathematical analysis on the other hand bring the essential questions of topographic self-organization to the point. Topographic self-organization is *not* just about minimizing an appropriate energy function, even if such energy functions may be devised. It was probably a piece of luck for research motivation that the original rule has not been derived from an energy function. Otherwise the fact that the energy function had be devised to create an organized map would have obscured the fact that topographically organized maps can be created by a much larger variety of dynamics than are defined by an energy function of a certain character.

It will be an interesting question for the future to determine how strong the conditions have to be to guarantee a certain degree of system organization.

3.4 Further Approaches for Dynamics Quantification

Energy and Liapunov functions as discussed above are measures based on the dynamics of the learning rule and the SOM learning rule may be modified in such a way that it becomes the gradient of some energy function. However, one could adopt here another view, namely looking at the SOM purely from the dynamics system view. One would then like the energy function to be derived from a given dynamical system and not from additional external interpretation of the system as a topology preserving system. Since the construction of energy functions is impossible for the general SOM, Spitzner and Polani (1998) used a different approach to condense the dynamics of a 1-dimensional SOM into a smaller number of parameters, based on a principle from synergetics (Haken 1983). It separates the dynamics into fast and slow subsystems (Mees 1981; Jetschke 1989). Applied to the 1-dimensional SOM, the method revealed that close to the fixed point of the dynamics a condensation of the essential dynamics into few relevant degrees of freedom or "order parameters" was not possible. However, this might be possible if also states far from the fixed point are taken into account. An indication that this view could be useful to formulate a quantification of (self-)organization not based on a topographic interpretation of the map is the hierarchical structure of the metastable states for the linear SOM (Erwin et al. 1992b). This view will be an interesting research field for the future.

3.5 Measures of Curvature

In (Alder et al. 1991) a "crinkleness" measure is defined for SOMs. It is restricted to Kohonen maps with A having rectangular grid topology. For every "inner" neuron of A (every neuron surrounded by neighbours in every dimension of A) a local deformation is calculated. The crinkleness measure then is given by averaging these local deformations.

The Discrete Version The local deformation is calculated in (Alder et al. 1991) as follows: We consider the distortion with respect to the k-th dimension of A. If A has $n_1 \times n_2 \times \cdots \times n_k \times \cdots \times n_r$ grid topology and $i \equiv (i_1, \dots, i_k, \dots, i_r)$ is an inner neuron (i.e. $i_k \in \{2, \dots, n_k - 1\}$), let $i^{\pm} = (i_1, \dots, i_k \pm 1, \dots, i_r)$, further $v_k^- := \mathbf{w}_i - \mathbf{w}_{i^-}$ and $v_k^+ := \mathbf{w}_{i^+} - \mathbf{w}_i$.

The local deformation $c(i)$ of neuron i is then given by

$$\begin{aligned} c(i) &= \frac{1}{r} \sum_{k=1}^{r} \left(1 - \frac{\langle v_k^-, v_k^+ \rangle}{|v_k^-| \cdot |v_k^+|}\right) \\ &= \frac{1}{r} \sum_{k=1}^{r} \left(1 - \cos \angle(v_k^-, v_k^+)\right) \\ &= \frac{1}{r} \sum_{k=1}^{r} (1 - \cos \phi_k) \ , \end{aligned} \tag{5}$$

where ϕ_k is the angle $\angle(v_k^-, v_k^+)$ between v_k^- and v_k^+. The geometric situation can be visualized as in Fig. 5.

The average of $c(i)$ on all inner neurons of A will be called μ_{ATA}. As μ_{ATA} assumes a rectangular grid as topology of A, it presupposes significantly more structure than other organization measures only assuming some graph structure on A and one could hope to relate this measure to some of the well known curvature measures of the continuous case. For this purpose

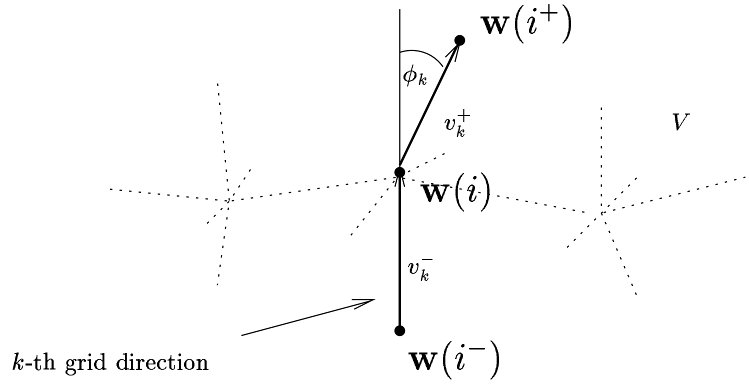

Fig. 5. Local deformation at a neuron

certain quantities of the discrete case must be converted to quantities of the continuous model.

To achieve this, define for given $i_1, \ldots, i_{k-1}, i_{k+1}, \ldots, i_r$ the function

$$\begin{array}{rcl} s : \{1, \ldots, n_k\} & \rightarrow & A \\ t & \mapsto & (i_1, \ldots, i_{k-1}, t, i_{k+1}, \ldots, i_r) \ . \end{array}$$

Then, if $i = s(t)$, obviously

$$\begin{aligned} v_k^+ &= [\mathbf{w} \circ s](t+1) - [\mathbf{w} \circ s](t) \\ v_k^- &= [\mathbf{w} \circ s](t) - [\mathbf{w} \circ s](t-1) \ . \end{aligned}$$

A Continuous Version To obtain the continuous version of the model, replace A, s and $\mathbf{w}$ by appropriate continuous versions of the corresponding sets and maps, thereby we are able to turn $\mathbf{w} \circ s$ into a smooth function $\psi : [0,1] \rightarrow V$; the small displacement v_k^+ becomes $\dot{\psi}(t)$ in the continuous version.

Now in the crinkleness measure the change of displacement vectors is measured in terms of $1 - \cos \phi_k$. To make the connection between the continuous and the discrete model and to obtain the differential analogy for $1 - \cos \phi_k$, we consider $\angle(\dot{\psi}(t), \dot{\psi}(t + \Delta t))$ instead of ϕ_k and investigate the Taylor expansion of $1 - \cos \angle(\dot{\psi}(t), \dot{\psi}(t + \Delta t))$ with respect to Δt around t. A somehow tedious calculation shows that the first non-vanishing coefficient of the expansion is that of Δt^2, i.e. the 2nd derivative of $1 - \cos \angle(\dot{\psi}(t), \dot{\psi}(t + \Delta t))$ with respect to Δt at $\Delta t = 0$ can be considered as the continuous version of the crinkleness at $\psi(t)$. It is given by

$$c(\psi(t)) = \frac{\langle \dot{\psi}(t), \dot{\psi}(t) \rangle \langle \ddot{\psi}(t), \ddot{\psi}(t) \rangle - \langle \dot{\psi}(t), \ddot{\psi}(t) \rangle^2}{\langle \dot{\psi}(t), \dot{\psi}(t) \rangle^2} \ . \tag{6}$$

Because of the Cauchy-Schwarz-inequality this term is always ≥ 0 (as is its discrete counterpart) and vanishes (this means local crinkleness 0) exactly when $\dot{\psi}(t)$ is parallel (or antiparallel) to $\ddot{\psi}(t)$, which means that change of the tangent takes only place in direction parallel (antiparallel) to the tangent.

In exactly this case $c(\psi(t))$ is minimal. Note that in this respect the continuous model differs from the discrete one, since in the latter v_k^- may be antiparallel to v_k^+, yielding a maximal crinkleness value, but in the continuous (smooth) case this cannot happen, since tangent vectors for t and $t + \Delta t$ are always close for small Δt.

This can be reformulated for a general non-vanishing vector field Z on the curve ψ (O'Neill 1983):

$$c_k(\psi(t)) = \left. \frac{\langle Z, Z\rangle\langle D_Z Z, D_Z Z\rangle - \langle Z, D_Z Z\rangle^2}{\langle Z, Z\rangle^2} \right|_{\psi(t)} , \tag{7}$$

where D denotes the canonical connection on V. Thus the differential geometric version of the crinkleness measure μ_{ATA} at location $\mathbf{w}_i \equiv \mathbf{w}(i) \in V$ is obtained by assuming A and V to be smooth manifolds of dimensions r and d, respectively, the latter furnished with a scalar product; then a collection $\{E_j | j = 1 \ldots r\}$ of vector fields on A is chosen forming a basis (orthonormal, if A is equipped with a scalar product) and setting:

$$c(\mathbf{w}(i)) := \sum_{j=1}^{r} c_j(D\mathbf{w}_i(E_j)) , \tag{8}$$

$D\mathbf{w}_i$ denoting the Jacobian of $\mathbf{w}$ at $i \in A$ in this context. The global crinkleness measure is then obtained by averaging over A, i.e. by integrating over A and normalizing afterwards.

Unfortunately this measure is not invariant with respect to the choice of the basis $\{E_j | j = 1 \ldots n\}$ (even when restricted to orthonormal ones), as can be shown by a straightforward example. Therefore it cannot be expressed as an abstract property of the embedding of a smooth manifold A into the smooth manifold V. This means that in the transition from the discrete to the smooth model, i.e. from the grid to the manifold the "special" character of certain selected directions of A is not lost. One would, however, prefer a measure taking advantage of the local isotropy of the smooth model and being insensible to the choice of a basis.

Possible Generalizations Through these considerations one is led to consider the possible derivation of a whole collection of crinkleness or – better – curvature measures for application to discrete SOMs from the well-known curvature notions of Riemannian geometry. One may apply the distinction between intrinsic curvature quantities measuring the "inner" distortion of the Kohonen embedding and quantities measuring the distortion of $\mathbf{w}(A)$ with respect to V. For $\mathbf{w}(A)$ having an "inner" distortion at least two dimensions are required, since the intrinsic curvature of a 1-dimensional manifold vanishes (O'Neill 1983). However, notions of the relative curvature of a submanifold embedded into a manifold also exist. Hence measures might be derived enabling to focus on different aspects of the embedding quality.

One should nevertheless keep in mind that these characterizations will be purely geometrical and restricted to evaluate the current map $\mathbf{w}$ without referring to the data manifold it is expected to describe. Thus, one obtains two possible informations by the measures: On condition that a SOM is an appropriate model for the given data manifold, the curvature measures give an information on the geometrical structure of the data manifold. In this case, large curvature values will have to be traced back to the form of the data manifold. But much more often large curvatures will be result of the well-known crinkling effects of nets where dimension of A is inappropriately chosen (as e.g. in Fig. 2(b)).

3.6 Similarity- and Metric-Based Measures

Goodhill et al. (1995); Goodhill and Sejnowski (1997a) discuss measures that are based essentially on notions of similarity. A measure of similarity can be realized by a metric, but need not fulfil the triangle inequality. In the mentioned papers, the similarity measures are realized as either a (often Euclidean) metric or as some monotonous functions applied to a metric Depending on the orientation of the similarity value, a good match is reflected by a low or a high value.

We cite a proposition from (Goodhill et al. 1995) that is useful for generalizing the notion of a topological homeomorphism to discrete spaces based on similarity measures. First, we first require a definition.

Definition 3. Given metric spaces $\langle X, d_X \rangle$ and $\langle Y, d_Y \rangle$, a map $M : X \to Y$ is called *similarity preserving* if

$$\begin{aligned} \forall x_1, x_2, x_3, x_4 \in X : d_X(x_1, x_2) < d_X(x_3, x_4) \Rightarrow \\ d_Y(M(x_1), M(x_2)) \leq d_Y(M(x_3), M(x_4)) \end{aligned} \tag{9}$$

Proposition 1. *Let $\langle X, d_X \rangle$ and $\langle Y, d_Y \rangle$ be identical metric spaces with countable dense subsets. If M is a bijection such that both M and M^{-1} are* similarity preserving*, then M is a (topographic) homeomorphism and X and Y are topologically equivalent via M.*

The similarity preservation condition is, as noted by Goodhill et al. (1995), stronger than required to guarantee homeomorphism, therefore the stronger notion of *topographic homeomorphism* is used. A naive definition of topology in discrete spaces is unsatisfactory because the discrete topology is trivial and makes all mappings continuous. The conditions of Proposition 1, however, make sense for discrete spaces, too, and can be used to define a nontrivial notion of topography preservation for mappings between discrete spaces.

A Measure for Topographic Homeomorphism In the following, we use our standard notation for input and output space also for the scenarios of Goodhill et al. Given a measure of similarity F_V on the input space and F_A on the output space, Goodhill et al. (1995); Goodhill and Sejnowski (1997a,b) define a measure C by[3]

$$C := \sum_{\substack{(i,j)\in A\times A\\ i\neq j}} F_A(i,j) F_V(\mathbf{w}_i, \mathbf{w}_j) \,. \tag{10}$$

Goodhill et al. (1995) show that minimizing C w.r.t. $\mathbf{w}$ yields a topographic homomorphism if it exists. They also point out that the measure C is related to quadratic assignment problems. Some special cases of the measure C are discussed in (Goodhill and Sejnowski 1997a). A measure very similar to the *inverted minimal distortion* introduced there has already been used in (McInerney and Dhawan 1994).

Further measures of map quality studied in (Goodhill and Sejnowski 1997a) are

Metric Multidimensional Scaling: introduced in (Torgerson 1952), given by

$$\sum_{\substack{(i,j)\in A\times A\\ i\neq j}} \big(d_A(i,j) - d_V(\mathbf{w}_i, \mathbf{w}_j)\big)^2 \,, \tag{11}$$

a low value denoting a good match;

Sammon measure: (Sammon 1969) a measure treating input and output space unsymmetrically via

$$\frac{1}{\sum\limits_{\substack{(i,j)\in A\times A\\ i\neq j}} d_A(i,j)} \sum_{\substack{(i,j)\in A\times A\\ i\neq j}} \frac{\big(d_A(i,j) - d_V(\mathbf{w}_i, \mathbf{w}_j)\big)^2}{d_A(i,j)} \,, \tag{12}$$

a low value denoting a good match;

Spearman coefficient: (Bezdek and Pal 1995), based on an order statistics (and not the numerical values) of the similarity values for the different (i,j) pairs. Let R_k and S_k enumerate the respective ranks of the values $d_A(i,j)$ and $d_V(\mathbf{w}_i, \mathbf{w}_j)$ for all the pairs $(i,j) \in A\times A$. Then the Spearman coefficient of this order statistics is given by

$$\frac{\sum_k (R_k - \overline{R})(S_k - \overline{S})}{\sqrt{\sum_k (R_k - \overline{R})}\sqrt{\sum_k (S_k - \overline{S})}} \tag{13}$$

[3] The notation used here differs slightly from that of the original papers, but is — apart from a constant factor 2 — essentially equivalent to that given there, assuming that the similarity measures are symmetrical in their arguments.

its value lies between 0 and 1, a high value denoting a good quality mapping. Its one of the measures mentioned in Sec. 2.1 that uses only the ranking information from the metrics of the spaces.

The Topographic Product The *topographic product* is a measure motivated by the study of dynamical systems that has been modified for use with SOMs.

The topographic product μ_{BP} as defined in (Bauer and Pawelzik 1992) is calculated as follows:

- For all $j \in A$ determine $n_1^A(j), n_2^A(j), \ldots, n_{N-1}^A(j) \in A$ such that

$$d_A(j, n_1^A(j)) \leq d_A(j, n_2^A(j)) \leq \cdots \leq d_A(j, n_{N-1}^A(j))$$

  and $n_1^V(j), n_2^V(j), \ldots, n_{N-1}^V(j) \in A$ such that

$$d_V(\mathbf{w}_j, \mathbf{w}_{n_1^V(j)}) \leq d_V(\mathbf{w}_j, \mathbf{w}_{n_2^V(j)}) \leq \cdots \leq d_V(\mathbf{w}_j, \mathbf{w}_{n_{N-1}^V(j)}) \ .$$

- For $j, k \in A$ set

$$Q_1(j,k) := \frac{d_V(\mathbf{w}_j, \mathbf{w}_{n_k^A(j)})}{d_V(\mathbf{w}_j, \mathbf{w}_{n_k^V(j)})}$$

  and

$$Q_2(j,k) := \frac{d_A(j, n_k^A(j))}{d_A(j, n_k^V(j)} \ .$$

- Set

$$P_3(j,k) := \left(\prod_{l=1}^{k} Q_1(j,l) Q_2(j,l) \right)^{1/2k} \ .$$

- The final measure is then given by the logarithmic average:

$$\mu_{\mathrm{BP}} := \frac{1}{N \cdot (N-1)} \sum_{j=1}^{N} \sum_{k=1}^{N-1} \log\bigl(P_3(j,k)\bigr) \ .$$

A value near 0 signifies good adaptation, negative values of μ_{BP} are expected to indicate folding of A into V (Bauer and Pawelzik 1992) (typically when "dimension" of A – considered as grid – is chosen too small), positive values are expected to indicate a topology mismatch in the other direction.

In the first step, the choice of $n_1^A(j), n_2^A(j), \ldots, n_{N-1}^A(j)$ need not be unique, when there are different pairings of neurons, such that e.g. $d_A(j,k) = d_A(j,k')$ with $k \neq k'$. No standard procedure is given in (Bauer and Pawelzik 1992) to resolve this ambiguity. Therefore different implementations of the

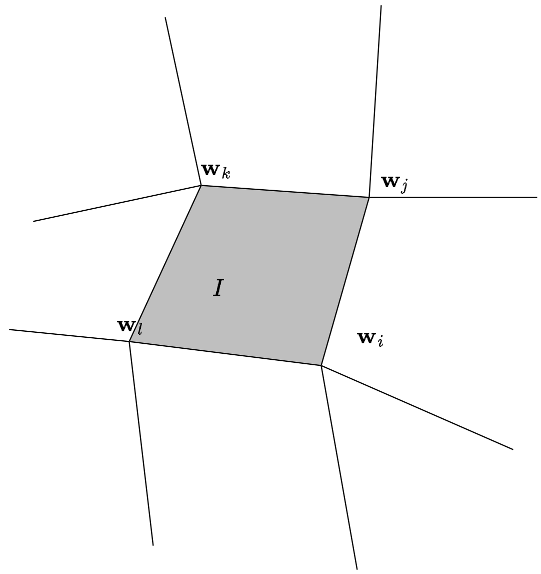

Fig. 6. A VBAR quadrilateral defined by four neurons in two-dimensional space

measure may yield different values for the intermediate values Q_1 and Q_2, while – empirically – the global result seems to be largely independent of these details[4].

3.7 A "Topological" Learning Rule

With (Hulle and Martinez 1993) and (Van Hulle 1997), the topological learning rules BAR and VBAR are introduced. They carry both the structural advantage of achieving or approximating an equiprobabilistic representation of the data manifold, thus maximizing entropy and, even more, being, in a sense, true topological learning rules.

The VBAR algorithm Here we give a short sketch of VBAR and refer the reader to (Hulle 1997, 2000) for more details. In VBAR, the output space is considered a rectangular grid of some given dimension d. Similar to the SOM, a neuron i has a corresponding "weight" vector $\mathbf{w}_i$ in the input space. Unlike in the SOM, however, the neurons do not just denote individual points to be mapped to the input space, but define the corners, and thus the borders of quadrilaterals H_k (d-dimensional rectangular intervals). Fig. 6 shows this for $d = 2$.

[4] The author's implementation of μ_{BP} has been compared to the implementation from (Speckmann et al. 1994).

In VBAR, an input signal is not considered to activate an individual neuron, but a complete quadrilateral. Exactly the neurons defining the corners of the respective quadrilateral will be updated. Let I define the image of a quadrilateral (multidimensional interval) under $\mathbf{w}$ in input space (Fig. 6). Let χ_I be the characteristic function of the set I, i.e.

$$\chi_I(x) := \begin{cases} 1 & \text{if } x \in I \\ 0 & \text{else .} \end{cases} \tag{14}$$

for all $x \in V$. For each neuron $i \in A$, let S_i be the set of those quadrilaterals that have i as corner. Then the VBAR learning rule is given by

$$\Delta \mathbf{w}_i(t) := \eta \sum_{I \in \mathbf{w}(S_i)} \chi_I(x) \, \mathrm{sgn}(x - \mathbf{w}_i(t)) \tag{15}$$

for every neuron i, where $x \in V$ is the current input, $\mathbf{w}(S_i)$ denotes the image of the quadrilateral set S_i under $\mathbf{w}$, i.e. the set of quadrilateral images under $\mathbf{w}$, η is the learning rate and sgn operates component-wise. For further details and the activation of quadrilaterals when x outside the grid map, see e.g. (Hulle 2000). For the VBAR algorithm, the notion of topographic order is well-defined.

Definition 4. A VBAR mapping is *topographically ordered* if for all inputs $x \in V$ the condition

$$\sum_I \chi_I(x) = 1 \tag{16}$$

holds where the sum is over all quadrilaterals I.

Condition (16) guarantees that, for a topologically ordered VBAR map, all points in V are covered by exactly one quadrilateral image $\mathbf{w}(I)$. For a point x that would not be covered, the term in (16) would become 0. A point x that would be covered multiply would return a number larger than 1. Thus, an organization measure could be defined based on the deviation of the term from (16) from unity for a given distribution of inputs x.

In addition to that, the VBAR rule also guarantees that, on convergence, the probability of activation of quadrilaterals is equidistributed, maximizing the entropy of the activation. Thus, in this context, the entropy could be used as (indirect) indicator of organization.

A "Topological" View of VBAR There is one property that makes the VBAR algorithm particularly interesting from the viewpoint of a topological mapping. As becomes clear throughout the present review, most measures of organization of topographic mappings are, in fact, not pure topological quantities. Most of them require a metric or at least a similarity structure on the input and output spaces. This is a stronger structural requirement than topology preservation (Sec. 3.6).

Even the predicate notion of Delaunay-topology preservation as in (Villmann et al. 1997) (see Sec. 3.8) requires a metric structure on the spaces, in particular a metric on V to construct the Delaunay graph, and two different metrics on A, depending on whether one considers the topology preservation of $\mathbf{w}$ or of its left inverse $\mathbf{i}^*$.

Here, this review wishes to direct the attention to a property particular to the VBAR model and the models directly related to it which, as far as known to the author, has not been pointed out before. Namely, the fact that the output space used in VBAR can be seen as a special case of using the topological notion of a *complex* (see e.g. (Henle 1979) or any other standard reference on algebraic topology). This review cannot give a full technical definition of a complex and only outlines it to make its point.

In algebraic topology, important notions are based on the study of d-dimensional simplices. For those, the notion of orientation and of boundary is defined. A d-dimensional complex is a structure that is constructed from d-dimensional simplices by topological identification (*gluing together*) of simplex boundaries. One of the simplest examples for a complex is a graph. It is constructed by 1-dimensional simplices (its edges), the boundaries of the edges are the vertices. An orientation is given by directing the edges. Higher-dimensional complexes can be seen as a generalization of that view by not only gluing edges together, but polygons, polyhedra and hyperpolyhedra to obtain the relevant structures.

The quadrangles used in VBAR can be constructed from simplices. They carry the full topological information about the structure of the output space, since they are truly d-dimensional, unlike the approaches restricted to graph or metric constructions to model higher dimensional spaces. It is therefore quite satisfying to see that in this model the topology preservation notion is simple to formulate. The VBAR model and its siblings can be seen as natural generalization of the discrete graph models of output space. It will be interesting to explore this type of generalization in the future.

3.8 Data-Oriented Measures

Intrinsic Distance Measure Kaski and Lagus (1996) introduce as measure the shortest mapped distance between the neurons whose weights are closest and second closest to a given data point in input space. More formally, let $x \in V$ be an input vector, $\mathbf{i}^*(x)$ be the neuron closest and $\mathbf{j}^*(x)$ the neuron second closest to the input (for simplicity, we assume uniqueness). Be further $\mathcal{S}_{i^*j^*}$ the set of paths starting at $\mathbf{i}^*(x)$ and ending at $\mathbf{j}^*(x)$ with edges from the Kohonen graph $\mathcal{C}_\mathrm{K}$. Then define the intrinsic distance as

$$\hat{d}(x) := d_V(x, \mathbf{w}_{\mathbf{i}^*(x)}) + \min_{S \in \mathcal{S}_{i^*j^*}} \sum_{(s_k, s_{k+1}) \in S} d_V(\mathbf{w}_{s_k}, \mathbf{w}_{s_{k+1}}) , \qquad (17)$$

where the paths $S \in \mathcal{S}_{i^* j^*}$ are represented as set of edges (s_k, s_{k+1}). The measure is then given by the expectation value $\mathbf{E}\big(\hat{d}(x)\big)$ of the intrinsic distance w.r.t. the data distribution.

$\mathbf{i}^*(x)$ and $\mathbf{j}^*(x)$ can be regarded as neurons that represent a given data point $x \in V$ "similarly" well in input space. In output space, however, they need not be close-by. One could have therefore taken the distance between $\mathbf{i}^*(x)$ and $\mathbf{j}^*(x)$ in output space as measure. Instead, in the approach chosen by Kaski and Lagus, the paths are projected back into input space. This can be interpreted as weighting the distance between both "representants" according to how large a region in data (input) space is in fact covered by the SOM. Thus, even if $\mathbf{i}^*(x)$ and $\mathbf{j}^*(x)$ seem far away in output space, they can still be close by in input space. The authors report the method to be more robust than that from (Villmann et al. 1994a). At the present time, a direct comparison of the measure to further organization measures is still an open task.

Measures Based on Delaunay Graphs The measure described in this section is based on the *Delaunay triangulation* of the set

$$\{\mathbf{w}_i | i \in A\} \equiv \mathbf{w}(A) \tag{18}$$

induced by the signal probability distribution on V. The mechanism applied is a Hebbian one as it is based on the simultaneous activation of neurons. The particular algorithm that enables determination not only of the Delaunay triangulation, but also of the structure of *2nd order Voronoi cells* of $\mathbf{w}(A)$ has been introduced in (Martinetz and Schulten 1993) and we will refer to it as the *Hebb-Martinetz-Schulten-* or *HMS-algorithm*[5].

A whole class of measures can be defined by making use of such a mechanism, which we will therefore call *Hebbian measures.* It is applied by construction of graphs as discrete models of data manifolds.

Voronoi Tessellation and Delaunay Triangulation Before we turn to the construction of the 2nd Voronoi triangulation by the Hebb algorithm of Martinetz and Schulten, we will redefine the notions of Voronoi cells and tessellations (consistently with Sec. 2.2) as well as the Delaunay triangulation.

Definition 5 (Voronoi Cell). Consider a SOM $\mathbf{w}$. The *Voronoi cell* (also *1st order Voronoi cell*) of a neuron $i \in A$ or the weight $\mathbf{w}_i \in \mathbf{w}(A)$ is the set

$$V_i := \{x \in V | \forall k \in A : d_V(x, \mathbf{w}_i) \leq d_V(x, \mathbf{w}_k)\} \ .$$

[5] We use this term also to distinguish it from the full *Self-Organizing Discrete Manifold* algorithm presented in (Martinetz and Schulten 1993), since the latter also involves a process distributing the $\mathbf{w}_i$, whereas in for our purposes it is applied to a given fixed $\mathbf{w}$.

The *2nd order Voronoi cell* of neurons i and j is the set

$$V_{ij} := \{x \in V | \forall k \in A \setminus \{i, j\} : d_V(x, \mathbf{w}_i) \leq d_V(x, \mathbf{w}_k) \wedge d_V(x, \mathbf{w}_j) \leq d_V(x, \mathbf{w}_k)\} .$$

Definition 6 (Voronoi Tessellation). Given a SOM $\mathbf{w}$, its *Voronoi tessellation* is the set

$$\{V_i | i \in A\}$$

of Voronoi cells V_i.

Definition 7 (Delaunay Triangulation, Hebb Graph). The *Delaunay triangulation* or *Delaunay graph* of a SOM $\mathbf{w}$ is a graph with vertex set A, i and j being adjacent iff V is an open subset of $\mathbb{R}^d$ and $\overline{V}_i$ and $\overline{V}_j$ have a common $d-1$-dimensional section. If i and j are adjacent for $\overline{V}_i \cap \overline{V}_j \neq \emptyset$, we speak of a *pseudo-Delaunay graph.*

The *weighted Delaunay* or *Hebb graph* of $\mathbf{w}$ induced by a probability distribution P (on V) is obtained by furnishing the edges (i, j) of the (simple) Delaunay graph with the weights $P(V_{ij})$, where $P(V_{ij})$ is the probability that an input signal lies in the 2nd order Voronoi cell V_{ij}. The edges of the Hebb graph are also called *Hebb connections.*

If V is a subset of $\mathbb{R}^d$, d_V being the Euclidean metric, then the Delaunay triangulation defines a triangulation of the space in the usual sense, except for degenerate choices of $\mathbf{w}$ (see (Okabe et al. 1992)).

The following general assumption will put us in the position to ignore pathological effects occurring at the boundaries of the Voronoi cells: From now on we will assume that $P(V_i \cap V_{i'})$ and $P(V_{ij} \cap V_{i'j'})$ always vanish for $i \neq i'$, $j \neq j'$, P being the probability distribution of input signals on V.

This assumption holds automatically if P has a density and d_V is the Euclidean metric e.g. on a subset of $\mathbb{R}^d$. However, it is not true in general if one of these conditions does not hold (Polani 1996). Our assumption ensures that we need not take such pathologies into consideration.

The Hebb Algorithm for the Self-Organizing Map The algorithm from (Martinetz and Schulten 1993, 1994) is recapitulated in the following. Note that the original algorithm has been modified insofar as to count the signals activating a connection and thus include a weight information about the Hebb connections. Let a SOM $\mathbf{w}$ be given. Then the HMS-algorithm is given by:

- For every adjacency pair $(i, j) \in \mathcal{C}_\mathrm{K} \subseteq A \times A$ let the *connection strength* be $c_{ij} := 0$.
- Choose randomly a finite set $S := \{x_1 \dots x_q\}$ of *Hebb signals* $x_1 \dots x_q \in V$ according to the probability distribution P.
- For every Hebb signal $x_l \in S$:

- Determine a neuron $i^* \in A$ minimizing $d_V(x_l, \mathbf{w}_{i^*})$ (a "best matching" neuron, typically $\mathbf{i}^*(x_l)$).
- Determine a neuron $j^* \in A \setminus \{i^*\}$ minimizing $d_V(x_l, \mathbf{w}_{j^*})$ (a "second best matching" neuron).
- Increment the connection strength $c_{i^*j^*}$ by 1.

If c_{ij}-values have been obtained by the above Hebb algorithm, c_{ij}/q then provide estimates for the $P(V_{ij})$-values and hence for the weights of the Hebb graph of $\mathbf{w}$ induced by P. The larger q and hence the set S is chosen, the better the estimate. At this stage there are several possibilities to calculate a quality measure for the Kohonen graph from the c_{ij}-values. Since they share the same vertex set A, the Kohonen graph can be compared directly to the Hebb graph. The Hebb measure μ_{H}, to be defined in Section 3.8, will be based on such a comparison. Villmann et al. also make use of the original (nonweighted) HMS-algorithm to calculate their organization measure.

A notion of Topology Preservation based on Delaunay triangulation Villmann et al. (1997) introduce a notion of topology preservation from the graph structure on A and the neighborhood structure of the Voronoi cells in V. Based on the notion of the pseudo-Delaunay graph, a notion of topology preservation has been defined by Villmann et al.. To distinguish it from other definitions, we call it Delaunay-topology preservation.

Definition 8 (Delaunay-topology preservation). Assume A is a rectangular lattice embedded into $\mathbb{R}^d$. Let d_A^1 represent the $\|.\|_1$ and d_A^∞ represent the $\|.\|_\infty$ norm (Sec. 2.3) on A. The map $\mathbf{w}$ is then called *Delaunay topology-preserving* iff $i, j \in A$ adjacent w.r.t. d_A^1 (i.e., for which $d_A^1(i,j) = 1$) are also adjacent as vertices of the pseudo-Delaunay graph and $\mathbf{i}^*$ is called *Delaunay topology-preserving* iff $i, j \in A$ adjacent as vertices of the pseudo-Delaunay graph are also adjacent w.r.t. d_A^∞, i.e. $d_A^\infty(i,j) = 1$.

Until now, the definition brought forward does not incorporate the structure of the data. However, the authors point out that it is essential to incorporate the structure of the data manifold, i.e. the support of the probability distribution in the calculation of the measures to obtain a quantity that adequately describes the quality of the mapping (this point has also been emphasized e.g. in (Kaski and Lagus 1996; Polani 1996)). In their model, Villmann et al. solve this problem by operating on an induced or *masked* Delaunay graph that depends on the data manifold. If M is the data manifold, the *masked* Voronoi cells are defined by $\tilde{V}_i = V_i \cap M$, where V_i are the standard Voronoi cells. The masked Delaunay graph is constructed from the masked Voronoi cells $\tilde{V}_i$ analogously to the nonmasked version by defining two neurons i and j as adjacent in the masked Delaunay graph iff $\overline{\tilde{V}}_i \cap \overline{\tilde{V}}_j \neq \emptyset$. The notion of topology preservation resulting from the masked Delaunay graph is the original version of the notion introduced in their paper.

Topographic Function In the categories from Sec. 2.1, the notion of Delaunay topology-preservation from Def. 8 acts as a predicate by determining whether or whether not a mapping is topology preserving. As is the case for many measures described here, e.g. for the "similarity match" measure C from Sec. 3.6, when the predicate is not fulfilled, one would like quantify the degree to which the observed map does not comply with the predicate. Instead of restricting to a single numerical value, Villmann et al. (1997) introduce a function that quantifies the structure of the mismatch.

Definition 9 (Topographic Function). Denote the metric defined by the masked Delaunay graph by d_D. Define for all $i \in A$, $k \in \mathbb{Z} \setminus \{0\}$ the functions $f_i : \mathbb{Z} \setminus \{0\} \to \mathbb{N}$ by:

$$f_i(k) := \begin{cases} |\{j \mid d_D(i,j) = 1, d_A^\infty(i,j) > |k|\}| & \text{for } k > 0 \\ |\{j \mid d_A^1(i,j) = 1, d_D(i,j) > |k|\}| & \text{for } k < 0 \;. \end{cases} \tag{19}$$

It gives the distribution of mismatches of a size beyond k for $\mathbf{w}$ and its left inverse $\mathbf{i}^*$. For $k > 0$, f_i gives the number of mismatches for the map $\mathbf{i}^*$ from V to A, for $k < 0$ the mismatches for the map $\mathbf{w}$ from A to V. Note that analogously to the definition of the topology preservation the required variant of d_A depends on which direction is considered, whether $\mathbf{i}^*$ or $\mathbf{w}$. The topographic function is then given by

$$\Phi(k) := \begin{cases} \frac{1}{|A|} \sum_{j \in A} f_j(k) & \text{for } k \neq 0 \\ \Phi(1) + \Phi(-1) & \text{for } k = 0 \;, \end{cases} \tag{20}$$

i.e. for $k \neq 0$ it is the value of the f_i averaged over all neurons.

The topographic function contains more information about the type of mismatch than the measures giving only a single number. First, it gives a direction of mismatch. If $\Phi(k) > 0$ for positive k, then this means that two neurons whose weights are close together in V (who are connected by a Delaunay edge) have a larger distance in A, i.e. that $\mathbf{i}^*$ is not Delaunay topology-preserving. This is typically the case if A has a too low dimension to accurately map V, as in Fig. 2. The largest k with nonzero $\Phi(k)$ indicates the scale size of the deviations. If k is large, then this indicates a deviation up to large size scales. Analogous statements hold for $k < 0$, where $\Phi(k) > 0$ indicates that $\mathbf{w}$ is not Delaunay topology-preserving and that the dimension of A is too high.

Note that to calculate the masked Delaunay graph to determine the topographic function in a concrete case, the authors use the original HMS-algorithm where it is only determined whether $P(V_{ij}) \neq 0$, i.e. whether the c_{ij} determined by the HMS-algorithm from Sec. 3.8 does not vanish.

A Hebbian Measure In (Böhme 1994; Polani 1996, 1997b,a), another measure is introduced and discussed that uses the HMS-principle to determine the Hebb (weighted Delaunay) graph with which the Kohonen graph may be compared. A comparison could be done by directly comparing the edges, e.g. counting the spare Kohonen edges (those Kohonen edges having no corresponding one in the Hebb graph) and vice versa. This would ignore the weights of the Hebb edges. However, such an indiscriminate comparison of the edges leads to sensitive discontinuities which are undesirable (Böhme 1994). This is illustrated by the standard example of a SOM with square net topology trained by an equidistribution on $[0,1]^2$ whose weights and receptive fields are shown in Fig. 7.

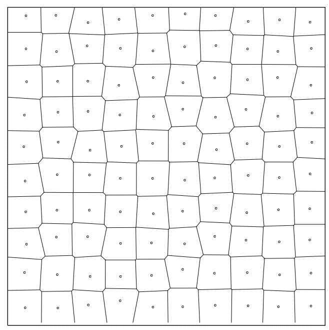

Fig. 7. Receptive fields of a SOM with square net topology, $V = [0,1]^2$ and P an equidistribution on V (Kohonen connections are not drawn).

Note that since P is an equidistribution in our example, $P(V_{ij})$ is given by the 2-dimensional volume of the 2nd order Voronoi cells V_{ij}; this volume in turn is nonzero only when the 1st order Voronoi cells V_i and V_j have a common edge (just fulfilling $V_i \cap V_j \neq \emptyset$ is not sufficient). The final state reached after a training is the average equilibrium state, i.e. of a state in which the weights $\mathbf{w}_i$ lie on slightly perturbed grid positions.

By inspection of Fig. 7 one can observe that even slight deviations from the symmetric equilibrium state of the SOM lead to "diagonal" edges in the Hebb graph for which no equivalent edges in the Kohonen graph are present. If comparison of Hebb and Kohonen graph were done ignoring the Hebb edges' weights, mismatch of a diagonal edge would be counted with the same significance as that of a rectangular edge. However, one would like the rectangular Kohonen still to be characterized as "well organized" when the $\mathbf{w}_i$ display some small deviations from the equilibrium grid positions. Moreover, even small perturbations may flip a diagonal edge (Fig. 8). Therefore even if at first correct diagonal Kohonen edges matching the Hebb edges were present, a small perturbation of $\mathbf{w}$ could transform those edges into spare ones, i.e. the resulting measure counting the matches would not be continuous.

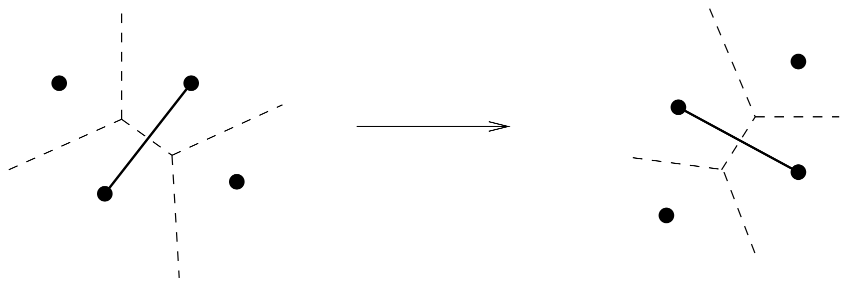

Fig. 8. Hebb edge flip induced by perturbation of $\mathbf{w}$ (deviation from square grid equilibrium positions is exaggerated for illustration)

Thus the demand for continuity leads us to take into account the weights of the Hebb edges since the diagonal edges have much smaller weights than the rectangular ones. A comparison of the graphs can be realized by furnishing the Kohonen edges with weights. This can be done in different ways, leading to similar results except for pathological cases. We will follow the conventions of (Böhme 1994), where the weight $\hat{c}_{ij}$ of a Kohonen graph edge $(i,j) \in \mathcal{C}_\mathrm{K}$ is set to

$$\hat{c}_{ij} := \hat{c} = \frac{\sum\limits_{(i,j)\in\mathcal{C}_\mathrm{H}} c_{ij}}{|\mathcal{C}_\mathrm{H}|} ,$$

i.e. to the average weight of the Hebb graph edges for all edges. The measure is now obtained by summing up the weights of Kohonen edges not matching any Hebb edges and vice versa and normalizing. Finally, the measure μ_H is calculated by subtracting the result from 1; a high degree of organization is therefore represented by a high value of $\mu_\mathrm{H}(\mathbf{w})$ since in this case there are only few non-matching edges. The formula for $\mu_\mathrm{H}(\mathbf{w})$ reads then[6]:

$$\begin{aligned}\mu_\mathrm{H}(\mathbf{w}) &:= 1 - \frac{\sum\limits_{(i,j)\in\mathcal{C}_\mathrm{K}\setminus\mathcal{C}_\mathrm{H}} \hat{c}_{ij} + \sum\limits_{(i,j)\in\mathcal{C}_\mathrm{H}\setminus\mathcal{C}_\mathrm{K}} c_{ij}}{\sum\limits_{(i,j)\in\mathcal{C}_\mathrm{K}} \hat{c}_{ij} + \sum\limits_{(i,j)\in\mathcal{C}_\mathrm{H}} c_{ij}} \\ &= 1 - \frac{\hat{c}\cdot|\mathcal{C}\setminus\mathcal{C}_\mathrm{H}| + \sum\limits_{(i,j)\in\mathcal{C}_\mathrm{H}\setminus\mathcal{C}} c_{ij}}{\hat{c}\cdot|\mathcal{C}| + \sum\limits_{(i,j)\in\mathcal{C}_\mathrm{H}} c_{ij}} . \end{aligned} \tag{21}$$

[6] For sake of simplicity in our notation we identify the values of $P(V_{ij})$ with their estimates c_{ij} obtained by the Hebb algorithm. Note that in those terms q is cancelled – it only plays a role for the accuracy of the c_{ij} as estimates for $p_{ij} \cdot q$.

4 Further Reading

This section will give a couple of pointers for further reading. The measures (Minamimoto et al. 1993) and (Demartines and Hérault 1995) are discussed in (Bauer et al. 1999). An organization measure related to C from Sec. 3.6 is introduced and used in (Mehler 1994). Demartines and Blayo (1992) use the variance of the connection lengths between weights in input space as a type of organization measure. This quantity is discussed e.g. in (Polani 1997b).

Different types of measures have been compared to each other in (Villmann et al. 1994a,b; Villmann 1996; Villmann et al. 1997; Villmann 1999; Bauer et al. 1999; Goodhill et al. 1995; Goodhill and Sejnowski 1997a,b; Polani 1997b, 1995, 1996). The last work, together with (Polani and Uthmann 1992, 1993; Polani 1997a, 1999) study the optimization of SOM topologies w.r.t. organization measures using GAs; it is found that this type of analysis can reveal much about the property of a given measure. In particular, for being able to claim that a given measure detects certain topological defects or favors a certain type of organization, that type of analysis is very helpful.

5 Summary

The present paper gave an overview over existing approaches to quantify the organization of SOMs and related topographic mapping models. The organization measures were discussed according to conceptual, structural and dynamical properties. In particular, the necessary properties relevant for the definition of organization measures were discussed. The overview shows clearly that organization measures can be defined from many conceptually different points of view, like information-theory, dynamical systems, topology, similarity, metrics or curvature. It also shows that the study of organization measures is generally regarded as central for the understanding of SOMs. And perhaps, in future, the study of this paradigmatic system will help to better understand the phenomena of self-organization in general.

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