A New Quantitative Measure of Topology Preservation in Kohonen's Feature Maps

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I. Introduction

The topology preservation map from a data manifold $M \subseteq V$ onto a lattice A of neural units i is one of the advantages of the Kohonen's self-organizing feature map (SOFM) (Kohonen 1984). This property can be used in a variety of information processing tasks, ranging from classification over robotics to data reduction and knowledge processing. To each neural unit i of A a reference or synaptic weight vector w_i is assigned, defining the receptive field or Voronoi polyhedron V_i of each unit i by the set of all data points $v \in M$ which are matched best by this reference vector. This mapping from the data manifold M onto the lattice A is called topology preserving, if neighbouring units i have receptive fields V_i which are adjacent on M. Under certain conditions, i.e., if a topological mismatch between M and A exists, the lattice folds itself into V and the topology preservation may be lost (Ritter et al. 1992).

The most known measure for characterizing the degree of topology preservation, the topographic product was introduced by (Bauer and Pawelzik 1992). Other methods are proposed by (Zrehen 1993), (Der et al. 1993). All these approaches do not use the data manifold itself for measuring and in this way they can provide correct results only for linear submanifolds $M \subseteq V$. If the manifold is nonlinear, like it is the case in many practical applications of SOFMs, all these approaches can not distinguish a correct folding due to the folded data manifold from a folding due to a topological mismatch between M and A. Particularly when using the SOFM for non-linear principle component analysis one has to have a means to distinguish between these two cases. In this paper we give a new approach for quantifying topology preservation using explicitly the structure of the data manifold. It can be applied to linear *and* non-linear data manifolds M. Further, this method allows to *quantify* the range of folds. Our approach employes what we call the topographic function, which is defined based on the so-called masked Voronoi polyhedra $\tilde{V}_i = V_i \cap M$ which were introduced in (Martinetz 1993) for defining neighbourhood and topology preservation of feature maps.

II. The Topographic Product applied to a SOFM

Kohonen's algorithm defines a self-organized feature map (SOFM) from a data manifold M embedded in a n_V-dimensional input space V onto a n_A-dimensional lattice A of neural units. With each time step a stimulus vector $v \in M$ is presented. The winner (best matching) unit i^* is defined by

$$\|w_{i^*} - v\|_V \leq \|w_i - v\|_V \quad \text{for all} \quad i \in A, \qquad (1)$$

with $\|\cdot\|_V$ denoting the Euclidean distance in V. The reference vectors w_i are adapted in a learning step according to

$$\triangle\, w_i = \epsilon h_{i^*,i}\,(v - w_i) \quad \text{for all} \quad i \in A, \qquad (2)$$

with the neighbourhood function

$$h_{i^*,i} = \exp\left(-\frac{\|i^* - i\|_A}{2\sigma^2}\right) \qquad (3)$$

determining the neighbourhood range in A. $\|\cdot\|_A$ denotes the Euclidean distance in A. ϵ and σ are learning parameters. The most known method for quantifying the topology preservation of a SOFM, the topographic product P, has been introduced by Bauer and Pawelzik (Bauer and Pawelzik 1992). It measures the preservation of the neighbourhood between the neural units i in A and their reference vectors w_i lying on M. However, the topographic product does not consider the neighbourhood relations of the reference vectors lying in M, but only the neighbourhood relations of the reference vectors within the embedding space V. Hence, an approach based on the topographic product is not able to differentiate between correct foldings arising from a nonlinear data manifold M and incorrect foldings which may result from a dimensional conflict between M and A or an incorrect formation of the map (topological defects, twists, kinks). An example to illustrate the problem is shown in Fig.1. In both the linear and nonlinear case of M the topographic product has the same value indicating a loss of topology preservation. However in the nonlinear case the map has been formed correctly.

III. The Topographic Function Φ_A^M

In this chapter we define the topographic function Φ_A^M for measuring the topology preservation of a SOFM, which considers explicitly the structure of the data manifold M. It was first introduced in (Villmann et al. 1994). Following (Martinetz 1993), we define the receptive field of a neural unit i by

$$R_i = V_i \cap M, \tag{4}$$

which corresponds to the masked Voronoi polyhedron $\tilde{V}_i$ in (Martinetz 1993). The basic idea of our approach is that we do not use the reference vectors w_i of the neural units i but their receptive fields R_i to measure neighbourhood relations. In a perfectly ordered SOFM only nearest lattice neighbours i' of a unit i have receptive fields $R_{i'}$ which are adjacent to R_i. If there are other units which have adjacent receptive fields, perfect topology preservation is lost. Let A be a $N_1 \times N_2 \times \ldots \times N_{n_A}$ neuron lattice of dimension n_A. Then neural unit i is indicated by $i = (i_1, \ldots, i_{n_A})$. For each unit i we define

$$f_i(k) = \#\{j \mid \|i-j\|_{\max} > k \; ; \; R_i \cap R_j \neq \emptyset\} \tag{5}$$

with $k = 1, \ldots, N_{\max}$, $N_{\max} = \max_{i=1}^{n_A} |N_i|$. $\#\{\cdot\}$ denotes the cardinality of a set and $\|\cdot\|_{\max}$ denotes the maximum norm. Looking at a neural unit i, $f_i(k)$ determines the number of units j which have receptive fields R_j adjacent to R_i and, at the same time, have a lattice distance to i larger than k. The topographic function is then defined by

$$\Phi_A^M(k) = \sum_{j \in A} f_j(k). \tag{6}$$

Φ_A^M is a monotonically decreasing function, and we obtain $\Phi_A^M \equiv 0$ if and only if the SOFM is perfectly topology preserving. The largest k for which $\Phi_A^M(k) \neq 0$ holds yields the range of the largest fold. As depicted in Fig.1 in the linear case we get $\Phi_A^M(k) \neq 0$ for all k-values, which indicates a mismatch over the range of the whole net. In the nonlinear case we obtain the correct result $\Phi_A^M(k) \equiv 0$.

Choosing a normalized k, i.e., $k^* = k/N_{\max}$, and choosing a normalized Φ_A^M, i.e.,

$$\Phi^{*M}_A = \Phi_A^M / N(N - 3^{n_A}) \tag{7}$$

with $N = \prod_{k=1}^{n_A} N_k$, allows to compare maps of different size.

IV. Computing the Topographic Function Φ_A^M

Computing Φ_A^M requires to determine whether two receptive fields R_i, R_j are adjacent on the given manifold M. A way to determine the adjacency of two receptive fields $R_i = V_i \cap M$, $R_j = V_j \cap M$ has been proposed in (Martinetz 1993). Let $\mathbf{C}$ be a connectivity matrix determining connections between units $i, j \in A$ (in addition to the connectivity matrix defined by the fixed lattice structure). Initially, the elements $\mathbf{C}_{ij}$ of $\mathbf{C}$ are set to zero. Simply by sequentially presenting input vectors $v \in M$ and each time connecting (setting $\mathbf{C}_{ij} = 1$) those two units i^*, j^*, the reference vectors w_{i^*} and w_{j^*} of which are closest and second closest to v, leads to a connectivity matrix $\mathbf{C}_{ij}$ for which

$$\lim_{t \to \infty} \mathbf{C}_{ij} = 1 \quad \Leftrightarrow \quad R_i \cap R_j \neq \emptyset \tag{8}$$

is valid. It can be shown (Martinetz 1993) that the resulting connectivity structure connects units and only units the receptive fields of which are adjacent. This allows to rewrite eq.(5) to

$$f_j(k) = \#\{i \mid \|i-j\|_{\max} > k \; ; \; \mathbf{C}_{ij} = 1\} \tag{9}$$

for k-values in the range of $k = 1, \ldots, N_{\max}$. After a SOFM has been formed, we then can determine Φ_A^M by the following algorithm:

1. present an input vector $v \in M$ and determine the two nearest reference vectors w_{i^*}, w_{j^*}.
2. connect the units i^*, j^*, i.e., set $\mathbf{C}_{i^*j^*} := 1$ and go to step 1 .

After a sufficient number of input vectors v the algorithm yields a connectivity matrix $\mathbf{C}$ for which eq.(8) is valid. $\mathbf{C}$ can then be used to calculate the topographic function Φ_A^M according to eq.(9) and eq.(6).

V. Comparison of the Topographic Function with the Topographic Product for Various Examples

We applied both the topographic function Φ_A^M and the topographic product to various examples of linear and nonlinear data manifolds. In the linear cases both approaches give the same result. In the nonlinear cases, however, only the topographic function yields a correct result.

At first we investigate the logistic map

$$x_{n+1} = x_n \lambda (1 - x_n) \tag{10}$$

The states (x_n, x_{n+1}) of the system form a nearly linear submanifold M_λ for small values of λ, but a nonlinear one otherwise. For various cases of λ we trained a chain of 64 neural units to represent M_λ. We compute both the topographic product and the topographic function and obtain in all cases $\Phi_A^M \equiv 0$. The topographic product P decreases with increasing λ

$$\begin{array}{rclcrcl} \lambda &=& 0.50: & P &=& 0.0009 \\ \lambda &=& 3.00: & P &=& -0.002 \\ \lambda &=& 3.95: & P &=& -0.015 \end{array} \qquad (11)$$

The negative values of P indicate an increasing dimensional conflict (Bauer and Pawelzik 1992), the submanifold, however, is real one-dimensional, i.e. there is not a dimensional conflict.

The results of the next test demonstrate that the stronger the nonlinearity is the lower is the value of P. As an example we take the twice iterated logistic map, i.e.

$$x_{n+2} = \lambda^2 x_n (1 - x_n)(1 - \lambda x_n (1 - x_n)) \qquad (12)$$

with $\lambda = 3.95$. The submanifold is now generated by the states (x_n, x_{n+2}) of the system. For $\lambda = 3.00$ and $\lambda = 3.95$ we get $P = -0.007$ and $P = -0.06$, respectively. The topographic function vanishes in both cases.

If a real dimensional conflict occurs, i.e. the map 'folds' itself into the input space, the topographic function indicates this situation very well. Moreover, it measures the scale of existing folds. As an example we consider the map from a squared input space onto a chain of 144 neural units. Then the chain folds itself into the input space like a Peano curve, as shown in Fig. 2. The topographic function shows the various length scales of the folds. The highest k-value k^* for which $\Phi_A^M(k) \neq 0$ indicates the longest range, and we find $k^* \approx 130$ (see Fig.2), i.e. the range includes nearly the whole chain. In the figure the k-values are not normalized. The topographic product yields $P = -0.07$ indicating also the dimensional conflict.

VI. Conclusion

We presented a novel approach to the problem of measuring the topology preservation of a SOFM. The approach is based on the neighbourhood relations between receptive fields. The introduced topographic function is an improvement over the topographic product suggested in (Bauer and Pawelzik 1992) since it determines the degree of topology preservation by considering explicitly the given input manifold M. This was demonstrated for various examples of nonlinear input manifolds.

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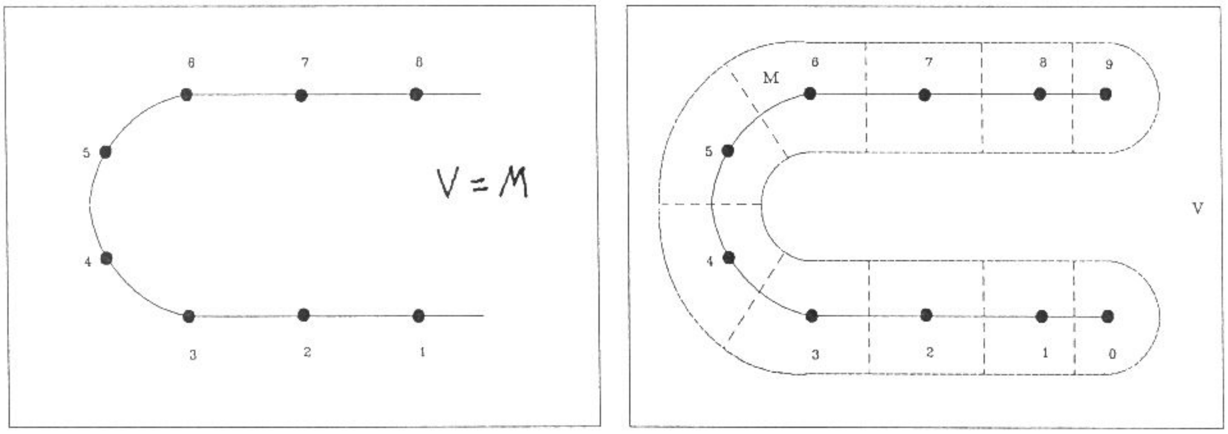

Figure 1: Example of a linear (left, $M = V$) and nonlinear (rightt, $M \subset V$) data manifolds with the hypothetical positions of the images of the neural units

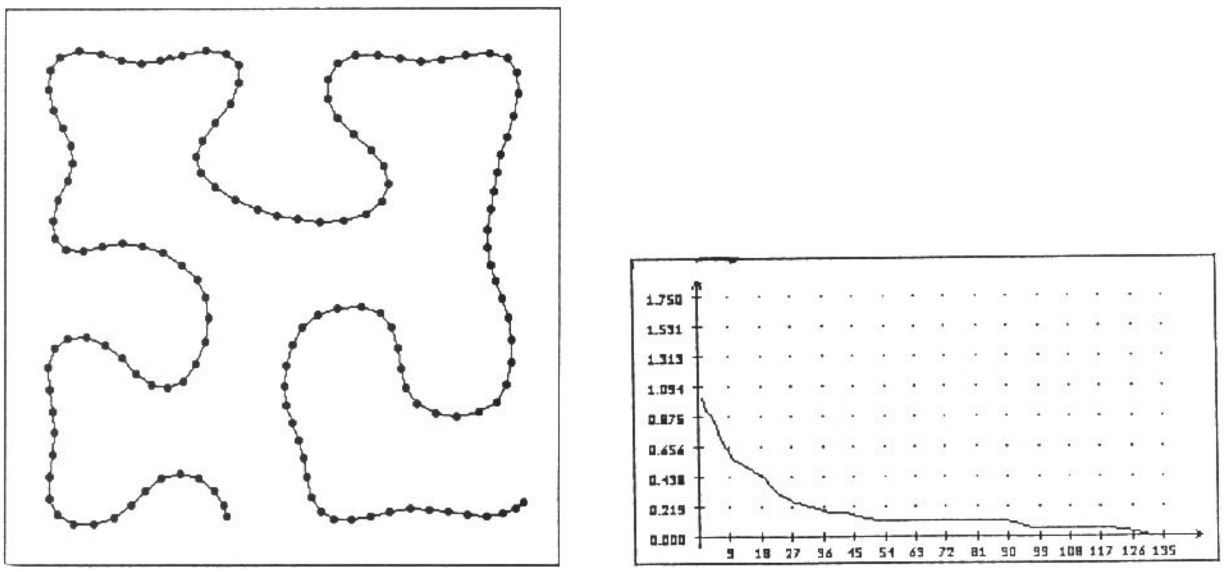

Figure 2: The topographic function for a map of a squared input space onto a chain of 144 neural units