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Topology Preservation in Self-Organizing
Feature Maps:
Exact Definition and Measurement

by

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1 Introduction

Based on a lattice A of N neural units $i \in A$, Kohonen's self-organizing feature map algorithm (SOFM) is able to form a topology preserving map $\mathcal{M}_A$ of a data manifold $M \subseteq \Re^d$ [1]. This property can be employed in a variety of information processing tasks, ranging from speech and image processing over robotics to data reduction and knowledge processing [2], [3], [4], [5], [6], [7], [8], [9], [10]. To each neural unit $i \in A$ a reference or synaptic weight vector $w_i \in \Re^d$ is assigned. The map $\mathcal{M}_A = (\Psi_{A\to M}, \Psi_{M\to A})$ of M formed by A is then defined by the mapping $\Psi_{M\to A}$ from M to A and the inverse mapping $\Psi_{A\to M}$ from A to M. These two mappings are determined by

$$\mathcal{M}_A = \begin{cases} \Psi_{M\to A} & : \quad M \longrightarrow A \quad ; \quad v \in M \longmapsto i^*(v) \in A \\ \\ \Psi_{A\to M} & : \quad A \longrightarrow M \quad ; \quad i \in A \longmapsto w_i \in M \end{cases} \tag{1}$$

with $i^*(v)$ as the neural unit with its synaptic weight vector $w_{i^*(v)}$ closest to v, i.e., with

$$\left\| w_{i^*(v)} - v \right\| \leq \| w_j - v \| \qquad \forall j \in A. \tag{2}$$

Starting from a fixed lattice structure A, Kohonen's self-organizing feature map algorithm distributes the synaptic weight vectors w_i such, that the map $\mathcal{M}_A$ of M formed by A is as topology preserving as possible. The reference vectors w_i are adapted in a learning step according to

$$\triangle\, w_i = \epsilon h_{i^*,i}\,(v - w_i) \quad \text{for all} \quad i \in A, \tag{3}$$

where $v \in M$ is the presented stimulus vector, $i^*(v)$ is defined again by eq.(2) and the neighborhood function

$$h_{i^*,i} = \exp\left(-\frac{\|i^* - i\|_A^2}{2\sigma^2}\right) \tag{4}$$

determines the neighborhood range in A by the choice of the radius σ. $\|\cdot\|_A$ denotes the Euclidean distance in A. ϵ is the learning parameter.

To what degree the topology is preserved depends on the choice of the lattice structure A. Depending on the form of the manifold M, a one-dimensional, two-dimensional, etc. lattice has to be chosen to obtain the best result. In most applications, however, the form of the manifold M is not known and, hence, it is not clear *a priori* which lattice structure one should choose. One has to try different lattice structures and has to determine somehow which lattice yields the highest degree of topology preservation.

Various qualitative and quantitative methods for characterizing the degree of topology preservation have been proposed [11], [12], [13], [14], [15]. However, non of these approaches take the form of the data manifold into the measurement and,

Abstract

The neighborhood preserving property of self-organizing feature maps like the Kohonen map is a useful quality of this algorithm. However, if a dimensional conflict arises this property is lost. Various qualitative and quantitative measures are known for determining the degree of topology preservation. They are based on using the locations of the synaptic weight vectors. This point of view may fail in case of non-linear data manifolds. To overcome this problem, in this paper we present an approach which uses the induced receptive fields for determining the degree of topology preservation. We first introduce a precise definition of what topology preservation means and then give a tool for measuring it, which we call the topographic function.The topographic function vanishes if and only if the map is topology preserving. We demonstrate the power of this tool for various examples of data manifolds.

is captured?

A reasonable definition for *neighborhood of reference vectors w_i, w_j on M* was given in [16], [17] based on the masked Voronoi polyhedra of w_i and w_j. Two *synaptic weight vectors w_i, w_j are adjacent on M* if and only if their receptive fields on M, determined by the masked Voronoi polyhedra $R_i = \tilde{V}_i$, $R_j = \tilde{V}_j$ with

$$\tilde{V}_i = \{v \in M \mid \|v - w_i\| \leq \|v - w_j\| \quad \forall\, j \in A\} \tag{5}$$

are adjacent, i.e., if and only if $R_i \cap R_j \neq \emptyset$. We remark that the definition of adjacency by the non-vanishing intersections makes sense, because the $\tilde{V}_i$ are defined as closed sets.

Two vertices $i = (i_1, \ldots, i_{d_A})$, $j = (j_1, \ldots, j_{d_A})$ of a rectangular d_A−dimensional lattice are adjacent in A if and only if they are nearest neighbors in the lattice A. A proper definition of the two neighborhood preservations, however, requires us to take into account both the nearest lattice neighbors based on the maximum-norm

$$\|\cdot\|_{\max} \overset{def}{=} \max_{j=1}^{d_A} \left|(\cdot)_j\right| \tag{6}$$

and the nearest lattice neighbors based on the Euclidean norm $\|.\|_E$, if we consider the positions of the neural units in the lattice as usual vectors. This is illustrated in Fig. (7), which shows a two-dimensional rectangular lattice representing a square. To be able to discern the adjacency of reference vectors w_i their receptive fields, i.e., their masked Voronoi polygons $\tilde{V}_i$, are depicted. Of course, the SOFM in Fig. (7) is topology preserving. Obviously, this requires vertices which are adjacent in the lattice according to the Euclidean norm $\|.\|_E$ or the summation-norm

$$\|\cdot\|_\Sigma \overset{def}{=} \sum_{j=1}^{d_A} \left|(\cdot)_j\right| \tag{7}$$

to be assigned to neighboring locations w_i. On the other hand, adjacent locations w_i have to belong to adjacent vertices. However, they do not necessarily have to belong to vertices which are adjacent according to the Euclidean norm $\|.\|_E$, which would be too strict, but only to vertices which are adjacent according to the maximum-norm $\|.\|_{\max}$. This leads us to the following definition of topology preservation of SOFMs with rectangular lattices:

Definition 2.1 *Let A be a d_A-dimensional rectangular lattice and M be a data manifold $M \subseteq \Re^d$. A map $\mathcal{M}_A = (\Psi_{A\to M}, \Psi_{M\to A})$ of M is topology preserving if both the mapping $\Psi_{M\to A}$ from M to A and the inverse mapping $\Psi_{A\to M}$ from A to M is neighborhood preserving.*

1. *The mapping $\Psi_{M\to A}$ is neighborhood preserving if and only if locations w_i, w_j which are adjacent on M belong to vertices i, j which are adjacent in A according to the* maximum-norm $\|.\|_{\max}$ *in A.*

hence, can provide correct results only for linear or nearly linear submanifolds $M \subseteq \Re^d$. If the manifold is nonlinear, as it is the case in many practical applications of SOFMs, non of these approaches can distinguish a correct folding due to the folded non-linear 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 (PCA) one has to have a means to distinguish between these two cases. In this paper we give a new approach for quantifying topology preservation which explicitly takes the structure of the data manifold into account. The approach, which employs what we call the *topographic function*, can be applied to linear *and* non-linear data manifolds M and, further, allows us to quantify the range of the folds.

In Section 2 we introduce a mathematical definition of topology preservation for rectangular lattices A, which in Section 3 leads to the so-called topographic function as a measure for the degree of topology preservation of a map $\mathcal{M}_A$ of M. It is shown how the topographic function can be evaluated by a simple mechanism based on the "competitive Hebbian rule", which was introduced in [16], [17]. In Section 4 we demonstrate via examples, ranging from the logistic map, over speech data to satellite images, the potential of the topographic function not only as a measure for the degree of topology preservation but as a general means for obtaining information about the dimensionality and structure of the data manifold M. The results are compared with the results provided by the so-called topographic product, which was proposed by [11] as an alternative method for measuring the degree of topology preservation. In the last section, we show how the mathematical definition of topology preservation for rectangular lattices can be generalized to arbitrary lattice structures.

2 A Definition of Topology Preservation for Rectangular Lattices

We want to call a map $\mathcal{M}_A = (\Psi_{A\to M}, \Psi_{M\to A})$ of M "topology preserving", if both the mapping $\Psi_{M\to A}$ from M to A as well as the inverse mapping $\Psi_{A\to M}$ from A to M is neighborhood preserving. Hence, to determine whether a SOFM is topology preserving we have to measure these two neighborhood preservations. To be able to measure these two neighborhood preservations we first have to define them. Per definition we regard the mapping $\Psi_{M\to A}$ from M to A as being neighborhood preserving if reference vectors w_i, w_j which are adjacent on M belong to vertices i, j, which are neighbors in A. On the other hand, the inverse mapping $\Psi_{A\to M}$ from A to M is neighborhood preserving if adjacent vertices i, j are mapped onto locations w_i, w_j which are neighbors on M. How can we define *neighborhood of vertices i, j in A* and *neighborhood of reference vectors w_i, w_j on M* in a way that the intuitive understanding of topology preservation of a SOFM is then defined by

$$\Phi_A^M(k) \stackrel{def}{=} \begin{cases} \frac{1}{N}\sum_{j\in A} f_j(k) & k>0 \\ \Phi_A^M(1)+\Phi_A^M(-1) & k=0 \\ \frac{1}{N}\sum_{j\in A} f_j(k) & k<0 \end{cases} \tag{10}$$

We obtain $\Phi_A^M \equiv 0$ and, particularly, $\Phi_A^M(0) = 0$ if and only if the SOFM is perfectly topology preserving.

The largest $k^+ > 0$ for which $\Phi_A^M(k^+) \neq 0$ holds yields the range of the largest fold if the effective dimension of the data manifold M is larger then the dimension d_A of the lattice A. This is depicted in Fig.3 and Fig.4. Fig.3 shows a map of a squared data manifold onto a chain of 100 neural units, together with their receptive fields. The folds are involved all over the whole chain and, hence, the topographic function vanishes only for k-values larger then $k^+ = 98$, as seen in Fig.4. On the other hand, the smallest $k^- < 0$ for which $\Phi_A^M(k) \neq 0$ holds yields the range of the largest fold if the effective dimension of the data manifold M is smaller than the dimension d_A of the lattice A. In this way the values k^+ and k^- give information about the degree of the dimensional conflict. Small values of k^+ and k^- indicate that there are only local dimensional conflicts,whereas large values indicate the global character of the dimensional conflict.

3.2 Evaluating the Topographic Function Φ_A^M

Calculating Φ_A^M requires to determine the induced Delaunay triangulation $\mathcal{D}_M$. A way to determine $\mathcal{D}_M$ has been proposed in [16], [17]. Let C be a connectivity matrix which determines connections between units $i,j \in A$ (in addition to the connectivity matrix defined by the fixed lattice structure). Initially, the elements $\mathbf{C}_{ij} \in \{0,1\}$ of $\mathbf{C}$ are set to zero. It can be shown that simply by sequentially presenting input vectors $v \in M$ and each time connecting those two units i^*, j^* (setting $\mathbf{C}_{i^*j^*} = 1$) the reference vectors w_{i^*}, w_{j^*} of which are closest and second closest to v, the connectivity matrix $\mathbf{C}$ converges to

$$\lim_{t\to\infty} \mathbf{C}_{ij} = 1 \quad \Leftrightarrow \quad R_i \cap R_j \neq \emptyset \tag{11}$$

[16], [17]. After a sufficient number of input vectors v have been presented, the connectivity matrix $\mathbf{C}$ connects units and only units i, j the receptive fields $R_i = \tilde{V}_i$, $R_j = \tilde{V}_j$ of which are adjacent and, hence, defines the induced Delaunay triangulation $\mathcal{D}_M$. With this algorithm we obtain the following scheme for determining the graph structure $\mathbf{C}$ of the Delaunay triangulation:

1. present an input vector $v \in M$

2. *The mapping $\Psi_{A\to M}$ is neighborhood preserving if and only if vertices i, j which are adjacent in A according to the* **Euclidean norm** $\|.\|_E$ *or the* **summation-norm** $\|\cdot\|_\Sigma$ *in A are assigned to neighboring locations w_i, $w_j \in M$.*

These definitions of neighborhood preservation are valid for the special but most widespread case of SOFMs based on rectangular lattices. How they can be generalized to arbitrary lattices is shown in the Appendix.

3 The Topographic Function Φ_A^M

3.1 Definition of the Topographic Function Φ_A^M

Let A be a $N_1 \times N_2 \times \ldots \times N_{d_A}$ rectangular lattice of dimension d_A. The lattice consists of $N = N_1 \times N_2 \times \ldots \times N_{d_A}$ neural units, and each unit i is indicated by $i = (i_1, \ldots, i_{d_A})$. To each i a reference vector is assigned which maps i onto a location w_i on the given data manifold M. As has been outlined in [16], [17], the masked Voronoi polyhedra in eq. (5) define the so-called induced Delaunay triangulation $\mathcal{D}_M$ of the set of w_i. The induced Delaunay triangulation is the graph which connects those and only those w_i, w_j which have adjacent masked Voronoi polyhedra $\tilde{V}_i$, $\tilde{V}_j$, i.e., which have adjacent receptive fields R_i, R_j on M. The induced Delaunay triangulation $\mathcal{D}_M$ defines a distance metric $\|.\|_{\mathcal{D}_M}$ between the w_i. The distance

$$d_{\mathcal{D}_M}(i,j) \stackrel{def}{=} \|w_i - w_j\|_{\mathcal{D}_M} \tag{8}$$

between two reference vectors is then determined by their shortest distance within the graph $\mathcal{D}_M$. Hence, two reference vectors w_i, w_j are adjacent on M according to our definition in Section 2 if and only if they are nearest neighbors in $\mathcal{D}_M$, i.e., if and only if $d_{\mathcal{D}_M}(i,j) = 1$. We can now define the *topographic function* Φ_A^M which is able to measure the topology preservation of a SOFM according to our definition. For each neural unit i we define

$$\begin{aligned} f_i(k) &\stackrel{def}{=} \#\{j \mid \|i-j\|_{\max} > k \; ; \; d_{\mathcal{D}_M}(i,j) = 1\} \\ f_i(-k) &\stackrel{def}{=} \#\{j \mid \|i-j\|_E = 1 \; ; \; d_{\mathcal{D}_M}(i,j) > k\} \end{aligned} \tag{9}$$

with $k = 1, \ldots, N-1$. $\#\{\cdot\}$ denotes the cardinality of a set. Looking at a neural unit i, $f_i(k)$ measures the neighborhood preservation of $\Psi_{M\to A}$, and $f_i(-k)$ measures the neighborhood preservation of $\Psi_{A\to M}$, as they have been defined in Section 2. The topographic function of the map $\mathcal{M}_A = (\Psi_{A\to M}, \Psi_{M\to A})$

For instance, if we map a squared input space onto a lattice of 16×16 neural units, we obtain $P = 0.0005$. We applied both the topographic function Φ_A^M and the topographic product P to various examples of linear and nonlinear data manifolds. In the linear cases both approaches gave the same result. In the nonlinear cases, however, only the topographic function provided correct results. If a real dimensional conflict occurs, i.e., the map 'folds' itself into the input space, the topographic function indicates this situation. Further, it is even able to measure the scale of existing folds. As an example we consider again the map from a squared input space onto a chain of 100 neural units. In this case the chain folds itself into the input space like a Peano curve, as shown in Fig.3. The topographic function reveals the various length scales of the folds. The highest k-value k^* for which $\Phi_A^M(k) \neq 0$ indicates the longest range. For our example we find $k^* = 98$ (see Fig.4), i.e., the range includes nearly the whole chain. The topographic product yields $P = -0.107$ which also indicates the dimensional conflict.

To demonstrate the difference between the topographic product and the topographic function in the case of non-linear data manifolds we first investigate the logistic map

$$x_{n+1} = x_n \lambda (1 - x_n) . \tag{13}$$

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 computed both the topographic product and the topographic function and obtained in all cases $\Phi_A^M \equiv 0$. The topographic product P, however, decreases with increasing λ

$$\begin{aligned} \lambda &= 0.50 : \quad P = 0.0009 \\ \lambda &= 3.00 : \quad P = -0.002 \\ \lambda &= 3.95 : \quad P = -0.015. \end{aligned} \tag{14}$$

The negative values of P indicate an increasing dimensional conflict (see eq.(12)), the submanifold, however, is still one-dimensional; i.e., there is no dimensional conflict. As second example we take the twice iterated logistic map, i.e.,

$$x_{n+2} = \lambda^2 x_n (1 - x_n) (1 - \lambda x_n (1 - x_n)) . \tag{15}$$

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 obtain $P = -0.007$ and $P = -0.06$, respectively. The topographic function vanishes in both cases.

Now we investigate a more realistic example. The satellites of LANDSAT-TM type produce pictures of the earth in 7 different spectral bands. The resolution is $30m \times 30m$ for the bands 1-5 and band 7. Band 6 has a resolution of

2. determine the nearest reference vector w_{i^*} and the second nearest reference vector w_{j^*}
3. connect the units i^*, j^*, i.e., set $C_{i^*j^*} := 1$
4. go to step 1 .

With this connectivity matrix C we are able to determine the distances $d_{\mathcal{D}_M}(i,j)$ between the reference vectors [18], which then allows us to calculate Φ_A^M according to (9) and (10).

4 Applications of the Topographic Function and Comparison with the Topographic Product

4.1 Comparison of the Topographic Function with the Topographic Product for Various Examples

Kohonen's algorithm defines a self-organizing feature map (SOFM) from a data manifold M embedded in a d-dimensional input space $\Re^d$ onto a d_A-dimensional lattice A of neural units. A method for quantifying the topology preservation of a SOFM is the topographic product P which was introduced by Bauer and Pawelzik [11]. It measures the neighborhood preservation of the mapping from the neural units i in A onto their reference vectors w_i. Thereby however, the topographic product does not take into account the shape of M, but considers only the neighborhood 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 which illustrates the problem is shown in Fig.1 and Fig. 2. 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.

In the linear case we get the following values for P, depending on whether d_A is smaller, equal to or larger then d [11]

$$\begin{aligned} P<0 &\quad \text{for} \quad d_A<d \\ P=0 &\quad \text{for} \quad d_A=d \\ P>0 &\quad \text{for} \quad d_A>d. \end{aligned} \tag{12}$$

4.2 Principal Component Analysis and the Topographic Function

The advantage of the SOFMs is that they can represent linear *and* non-linear data manifolds in the sense of principle component analysis (PCA). In this section we want to use the topographic function as a tool to control the evaluation of a SOFM for PCA of a possibly non-linear data manifold M. We discuss the case of a linear data manifold $M \subseteq \Re^d$ with the probability density $p(M)$ and $\tilde{M} \subset M$ as a nonlinear submanifold with $1 \geq p(v) \gg 0$ if $v \in \tilde{M}$ and $0 < p(v) \ll 1$ if $v \in M \backslash \tilde{M}$. The map folds itself into $\tilde{M}$ because of the higher probability density in $\tilde{M}$. Furthermore, we assume that the choice of the structure (connectivity graph $\mathbf{C}^A$) of the used lattice A is in agreement with the structure of $\tilde{M}$. The task is to minimize the description error

$$\rho = \max_{v \in M} \left\| v - w_{i^*(v)} \right\| \tag{16}$$

with $i^*(v)$ as defined in eq.(2) under the condition that the map $\mathcal{M}_A = (\Psi_{A \to M}, \Psi_{M \to A})$ of M formed by A as introduced in eq.(1) is topology preserving. If the topographic function indicates a loss of the topology preserving property during the learning process, which is coupled with the annealing algorithm for the parameter σ of the neighborhood function in eq.(4), one have to increase the value of σ again.

The map folds itself into $\tilde{M}$ because of the higher probability density in $\tilde{M}$. However, if we compute Φ_A^M as defined above it will indicate the folds as topological defects although in the sense of a PCA the map is correctly formed. We can overcome this problem by introducing the induced receptive fields of high probability

$$R_j^h = R_j \cap \tilde{M} \tag{17}$$

of neuron j. Now the idea is the same as above. We determine the non-vanishing intersections of the R_j^h to compute

$$\Phi_A^{\tilde{M}} = \Phi_A^M \Big|_{\tilde{M}} . \tag{18}$$

In practice we compute the connectivity matrix $\mathbf{C}_{ij}$ with respect to the R_j. In addition to the usual algorithm we introduce a suitable chosen maximal age $a_{\mathbf{max}}$ of a connection $\mathbf{C}_{ij}$. For instance, we choose $a_{\mathbf{max}} = N/p_{\min}$ where N is the number of neural units and $p_{\min}$ is the minimum of $p(v)$ for all $v \in M$. In every time step the age a_{i^*j} of all existing connections of the best matching unit i^* is increased. The age $a_{i^*j^*}$ of the new connection $\mathbf{C}_{i^*j^*}$ of the two best matching units is set to zero. Connections $\mathbf{C}_{i^*j}$ with an age higher than the maximal age $a_{\mathbf{max}}$ will be removed. This idea was first used in [16], [17] to compute the Delaunay triangulation of a "Neural-Gas-Network" in a parallel step during the evaluation of the net. With this algorithm we get the following scheme for determining $\Phi_A^{\tilde{M}}$:

$60m \times 60m$ only. The spectral bands represent useful domains of the whole spectrum in order to detect and discriminate vegetation, water, rock formations and cultural features [19], [20]. The spectral information associated with each pixel of a LANDSAT scene is represented by a vector $v \in \Re^d$ with $d = 7$, the number of spectral bands. Because of the rougher resolution of band 6 this channel is often dropped. Hence, the LANDSAT data may be represented as clouds of data points in a 6-dimensional space. The aim of any classification algorithm is to subdivide this data space into subsets of data points which belong to a certain category corresponding to a specific feature like wood, industrial region, and so on, each feature being specified by a certain prototype data vector. An approach with self-organizing feature maps has been successfully applied for instance in meteorology (cloud detection) [21] and earth surface clustering of Kuwait [22].

One way to get good results for visualization is to use a SOFM dimension $d_A = 3$. Then we are able to interprete the positions of the neurons in the *three*-dimensional neuron lattice A as a vector $c = (r, g, b)$ in the color space C, where r, g, b are the intensity of the colors red, green and blue. This assigns colors to categories (winner neurons) so that we end up immediately with the pseudo color version of the original picture for visual interpretation [23]. However, since we are mapping the data clouds from a 6-dimensional input space onto a *three*-dimensional color space there may arise dimensional conflicts and the visual interpretation may fail. Therefore, we tested lattices with the dimensions $d_A = 2, 3$ with 16×16 and $7 \times 6 \times 6$ neural units, respectively, to see whether they are topology preserving according to both the topographic product and the topographic function. In the three-dimensional case both the topographic product and the topographic function indicate mismatches. The topographic product yields $P = 0.09$. The topographic function is plotted in Fig.5 (points as $\diamond$). In case of the two-dimensional lattice of neural units we get for the topographic product $P = 0.002$, which suggests to prefer this configuration. However, the topographic function still indicates mismatches, as shown in Fig. 5 (points as $*$). This demonstrates that a visual interpretation of the results without a detailed consideration of the topology preserving property of the SOFM is misleading.

Finally, we discuss, again in comparison to the topographic product, the application of our approach to a set of speech data from the DPI-database of the III. Physikalisches Institut, Universität Göttingen, Germany. The data preprocessing is described in [24]. Here we remark only that the 4500 feature vectors represent a data submanifold lying in a 19-dimensional input space. We applied a *two*- and a *three*-dimensional SOFM to the data manifold, because the topographic product in the two-dimensional case is smaller than zero and in the three-dimensional case larger than zero. The topographic function for both cases is shown in Fig.6. In agreement with [11] we obtain that in both cases the topology preservation of the map is not perfect. Further, the topographic function indicates that it is not clear which lattice should be preferred.

Definition 5.1 *Suppose A to be a network of N neurons which are situated at points $i = (i_1, \ldots, i_{d_A}) \in \Re^{d_A}$ with reference or synaptic weight vectors $w_i \in M \subseteq \Re^d$. The connectivity graph $\mathbf{C}^A$ of A defines the structure of A. Let furthermore $\mathbf{C}^A(i)$ denote $\mathbf{C}^A$ where the neural unit i was taken as root. A (discrete) topology $\mathcal{T}_A^+(i)$ is induced by the graph metric in $\mathbf{C}^A(i)$. $\mathcal{T}_A^+(i)$ is said to be the* **strong neighborhood topology in A with respect to** *i, and $\left(A, \mathcal{T}_A^+(i)\right)$ is a topological space.*

Definition 5.2 *Consider for the moment A to be a set of points in $\Re^{d_A}$. Let $\mathcal{V}$ be the Voronoi diagram of $\Re^{d_A}$ with respect to A and $\mathcal{D}_A$ be its dual, the Delaunay graph. Let furthermore $\mathcal{D}_A(i)$ denote $\mathcal{D}_A$ where the neural unit i was taken as root. $\mathcal{D}_A(i)$ is equipped with the graph metric that in turn induces the (discrete) topology $\mathcal{T}_A^-(i)_M$ in $\mathcal{V}$ and, hence, also in A. $\mathcal{T}_A^-(i)$ is said to be the* **weak neighborhood topology in A with respect to** *i, and $\left(A, \mathcal{T}_A^-(i)\right)$ is a further topological space defined on the set A.*

Remark 5.1 *In the case of a rectangular lattice the weak neighborhood topology $\mathcal{T}_A^-(i)$ is weaker then the strong neighborhood topology $\mathcal{T}_A^+(i)$ also in the sense of mathematical topology [27], [28].*

In the next step we introduce a topology in the set of the synaptic weight vectors on the basis of their receptive fields, which again allows us to describe the neighborhood relationships between two vectors.

Definition 5.3 *Let $\Psi_{A\to M} : A \longrightarrow M^A \subset M \subseteq \Re^d$ be a map attributing to each neuron i a specific vector $w_i \in M^A$ with $M^A = \left\{w_i \in \Re^d \mid i \in A\right\}$. Furthermore, let $\mathcal{V}_M$ be the induced Voronoi diagram of M with respect to M^A. Let $\mathcal{G}_M$ be the dual Delaunay graph of $\mathcal{V}_M$. Let furthermore $\mathcal{G}_M(i)$ denote $\mathcal{G}_M$ where the neural unit i was taken as root. A (discrete) topology $\mathcal{T}_A^+(i)$ with respect to $i \in A$ is induced by the graph metric in $\mathcal{G}_M(i)$. $\mathcal{G}_M(i)$ is equipped with the graph metric that in turn induces the local (discrete) topology $\mathcal{T}_{M^A}(i)$ in $\mathcal{G}_M(i)$ and, hence, also in M^A. $\mathcal{T}_{M^A}(i)$ is said to be the* **$\Psi_{A\to M}$–induced neighborhood topology with respect to** *i in M^A and $\left(M^A, \mathcal{T}_{M^A}(i)\right)$ is a topological space.*

Now topology preservation of a map can be expressed by the following definition:

Definition 5.4 *The map $\mathcal{M}_A = (\Psi_{A\to M}, \Psi_{M\to A})$ is said to be* **topology preserving** *if both $\Psi_{M\to A} : \left(M^A, \mathcal{T}_{M^A}(i)\right) \longrightarrow \left(A, \mathcal{T}_A^-(i)\right)$ and $\Psi_{A\to M} : \left(A, \mathcal{T}_A^+(i)\right) \longrightarrow \left(M^A, \mathcal{T}_{M^A}(i)\right)$ are continuous maps of the respective topological spaces for all neural units $i \in A$ where $\Psi_{M\to A} : \Re^d \supseteq M \longrightarrow A$ is defined by $i(v) = \arg\left(\min_{i\in A} \|v - w_i\|\right)$. Irrespective of the different topologies $\Psi_{M\to A}$ is the inverse mapping of $\Psi_{A\to M}$.*

1. present an input vector $v \in M$
2. determine the nearest reference vector w_{i^*} and the second nearest reference vector w_{j^*}
3. increase the age a_{i^*j} for all j for which $C_{i^*j} = 1$ holds
4. connect the units i^*, j^*, i.e., set $C_{i^*j^*} := 1$ and $a_{i^*j^*} := 0$
5. set $C_{i^*j} := 0$ if $a_{i^*j} > a_{\max}$
6. go to step 1 .

Using this connectivity matrix $\mathbf{C}$ we are able to determine the distances $\|w_i - w_j\|_{\mathcal{D}_M}$ between the reference vectors [18], which then allows us to calculate Φ_A^M according to (9) and (10).

5 A Definition of Topology Preservation for Arbitrary Lattices

In this section we give a definition of Topology Preservation for Arbitrary Lattices. The basic idea is to describe the property of topology preservation in terms of the mathematical topology. The property of topology preservation of a map may then be based on the continuity of this map between topological spaces.

The induced Voronoi diagram $\mathcal{V}_M$ of a subset $M \subseteq \Re^d$ and its dual, the Delaunay graph (Voronoi graph) $\mathcal{D}_M$ with respect to a set $S = \{w_1, \ldots, w_N\}$ of points $w_i \in M \subseteq \Re^d$, is given by the masked Voronoi polyhedra

$$\tilde{V}_i = \{x \in M \mid \|x - w_i\| \leq \|x - w_j\| \quad j = 1 \ldots N, \quad j \neq i\} \tag{19}$$

as shown in [16], [17]. We remark that the Voronoi polyhedra are closed sets. The cells form a complete partitioning of M in the sense that $M = \cup_{i=1}^{N} \tilde{V}_i$. The induced Voronoi diagram $\mathcal{V}_M$ uniquely corresponds to its Delaunay graph $\mathcal{D}_M$ [25]. Two Voronoi cells $\tilde{V}_i$, $\tilde{V}_j$ are connected in $\mathcal{D}_M$ if and only if the intersection of it is non-vanishing, i.e., $\tilde{V}_i \cap \tilde{V}_j \neq \emptyset$ [25], [26]. Now we can define in $\mathcal{D}_M$ a graph metric as the minimal path length in the graph. In the general case the Voronoi diagram $\mathcal{V}$ of $\Re^d$ with respect to S is given by the Voronoi cells defined by

$$V_i = \left\{x \in \Re^d \mid \|x - w_i\| \leq \|x - w_j\| \quad j = 1 \ldots N, \quad j \neq i\right\} \tag{20}$$

Using the concepts introduced above we are now able to define in general terms what topology preservation for arbitrary lattices A with the connectivity graph $\mathbf{C}^A$ means.

By analogy to section 3.1 we define two kinds of neighborhood in the lattice A, but now as abstract topological definitions:

Remark 5.2 *We obtain* $\Phi_A^M \equiv 0$ *and, particularly,* $\Phi_A^M(0) = 0$ *if and only if the SOFM is perfectly topology preserving. The largest* $k^+ > 0$ *for which* $\Phi_A^M(k^+) \neq 0$ *holds yields the range of the largest fold if the effective dimension of the data manifold* M *is larger than the dimension* d_A *of the lattice* A*. The smallest* $k^- < 0$ *for which* $\Phi_A^M(k) \neq 0$ *holds yields the range of the largest fold if the effective dimension of the data manifold* M *is smaller then the dimension* d_A *of the lattice* A*. Small values of* k^+ *and* k^- *indicate that there are only local conflicts, whereas large values indicate a global dimensional conflict.*

Kohonen gave a definition for of what it means for a topographic map to be *ordered*, which finally should be discussed in the light of the definition studied in this paper. The following definition, only valid for the one-dimensional case was introduced in [29]:

Definition 5.5 *We consider a chain of* N *neural units* i *with weight vectors* w_i *and receptive fields* $R_i = \tilde{V}_i$ *as defined in 5. Let* $\eta_i(v)$ *be an activity function of the ith neuron with respect to a stimuli vector* $v \in M \subseteq \Re^d$*, for instance the negative distance* $-\|w_i - v\|$ *or the inverse distance* $\left(\frac{1}{\|w_i - v\|}\right)$*. Let* $X = \left\{x_j \in M \subseteq \Re^d \mid j = 1, \ldots, n\right\}$ *be a set of points, such that* $x_1 \overset{Rel}{\circ} x_2 \overset{Rel}{\circ} x_3 \overset{Rel}{\circ} \ldots \overset{Rel}{\circ} x_n$ *and for all neural units* i *exists a* $x_j \in X$ *for which* $x_j \in R_i$ *holds. The* $\overset{Rel}{\circ}$ *is an arbitrary suitably chosen relation, not necessarily transitive. The system is said to implement a* one–dimensional ordered mapping *if for* $i_1 > i_2 > i_3 > \ldots$

$$\begin{aligned} \eta_{i_1}(x_1) &= \max\nolimits_{i=1,\ldots,N} \eta_i(x_1) \\ \eta_{i_2}(x_2) &= \max\nolimits_{i=1,\ldots,N} \eta_i(x_2) \\ \eta_{i_3}(x_3) &= \max\nolimits_{i=1,\ldots,N} \eta_i(x_3) \\ &\vdots \\ &\text{etc.} \end{aligned} \tag{26}$$

holds.

We have given in this paper an explicit order relation $\overset{Rel}{\circ}$ based on an underlying topology, in contrast to the requirement of the existence of such a relation. The proposed straight–forward generalization of definition (26) to higher dimensions is (as pointed out in [30]) by no means trivial. In fact, one needs to make the relation $\overset{Rel}{\circ}$ more explicit in order to find whether definition (26) is applicable to higher–dimension, too. In this sense we gave the justification for Kohonen's early and not yet otherwisely worked out frame work, although the starting point of our investigation was the desire to improve the methods proposed in [11].

We have immediately the following two corollaries for the most important cases of rectangular and hexagonal (triangular) lattices:

Corollary 5.1 *In the case of a rectangular d_A-dimensional lattice A of neurons the strong topology is induced by the Euclidean norm $\|\cdot\|_E$ in A or the summation-norm $\|\cdot\|_\Sigma = \sum_{j=1}^{d_A} \left|(\cdot)_j\right|$, and the weak topology is induced by the maximum-norm $\|\cdot\|_{\max} = \max_{j=1}^{d_A} \left|(\cdot)_j\right|$. The systems of open sets $\mathcal{S}_\Sigma(i)$ and $\mathcal{S}_{\max}(i)$ defining the topologies $\mathcal{T}_A^+(i) = \mathcal{T}_A^\Sigma(i)$ and $\mathcal{T}_A^-(i) = \mathcal{T}_A^{\max}(i)$ are determined by*

$$\mathcal{S}_\Sigma(i) = \{s_k \mid s_k = \{l \in A \mid \|i-l\|_\Sigma = k \geq 1\}\} \tag{21}$$

and

$$\mathcal{S}_{\max}(i) = \{s_k \mid s_k = \{l \in A \mid \|i-l\|_{\max} = k \geq 1\}\}, \tag{22}$$

respectively.

Corollary 5.2 *In the special case of A being a hexagonal (triangular) lattice the weak and strong topology coincide. Hence, the definition of topology preservation relies on a single topology in the net which corresponds to the strong neighborhood topology.*

The conclusion in corollary 5.2 is in agreement with the definition of neighborhood given in [17]. By means of the definitions 5.1, 5.2, 5.3 and 5.4 we can now generalize the definition of the topographic function given in the equations (9) and (10). For each unit i we define

$$\begin{aligned} f_i(k) &\stackrel{def}{=} \#\left\{j \mid d_{\mathcal{T}_A^-(i)}(i,j) > k \; ; \; d_{\mathcal{T}_{MA}(i)}(i,j) = 1\right\} \\ f_i(-k) &\stackrel{def}{=} \#\left\{j \mid d_{\mathcal{T}_A^+(i)}(i,j) = 1 \; ; \; d_{\mathcal{T}_{MA}(i)}(i,j) > k\right\} \end{aligned} \tag{23}$$

with $k = 1, \ldots, N-1$. $\#\{\cdot\}$ denotes the cardinality of the set and

$$d_{\mathcal{T}(i)}(i,j) \stackrel{def}{=} \|w_i - w_j\|_{\mathcal{T}^\circ(i)} \; . \tag{24}$$

is a distance measure based on the topology $\mathcal{T}^\circ(i)$. Looking at a neural unit i, $f_i(k)$ with $k > 0$ determines the continuity of $\Psi_{M\to A}$ and $f_i(k)$ with $k < 0$ determines the continuity of $\Psi_{A\to M}$ as defined above. The topographic function of the neural lattice A with respect to the input manifold M is then in analogy to definition (10), again defined as

$$\Phi_A^M(k) \stackrel{def}{=} \begin{cases} \frac{1}{N}\sum_{j\in A} f_j(k) & k > 0 \\ \Phi_A^M(1) + \Phi_A^M(-1) & k = 0 \\ \frac{1}{N}\sum_{j\in A} f_j(k) & k < 0 \end{cases} \tag{25}$$

in analogy to section 3.1 we remark:

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A further issue is the topology preservation of the map $\Psi_{A \to M}$ which has been pointed out to be crucial as well for a strict definition of the intuitive notion of topology preservation.

6 Conclusion

We presented a novel approach to the problem of measuring the topology preservation of a SOFM. The approach is based on the neighborhood relations between receptive fields. The introduced topographic function is an improvement over the topographic product suggested in [11] 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. Furthermore we developed a general definition of topology preservation for SOFM's, based on topological spaces. It turns out that this definition is a generalization of a definition which has been proposed by Kohonen for the one-dimensional case.

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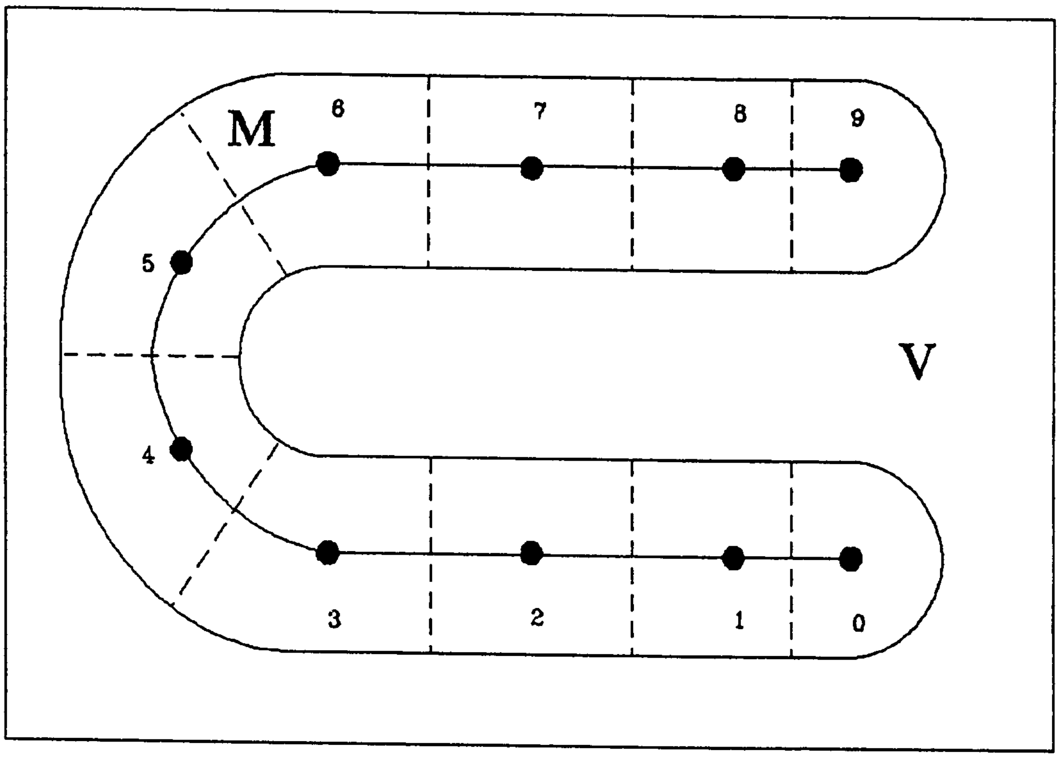

Figure 2: Example of a nonlinear ($M \subset V$) data manifold together with the hypothetical positions of the images of the neural units. The induced receptive fields are drawn by dashed lines.

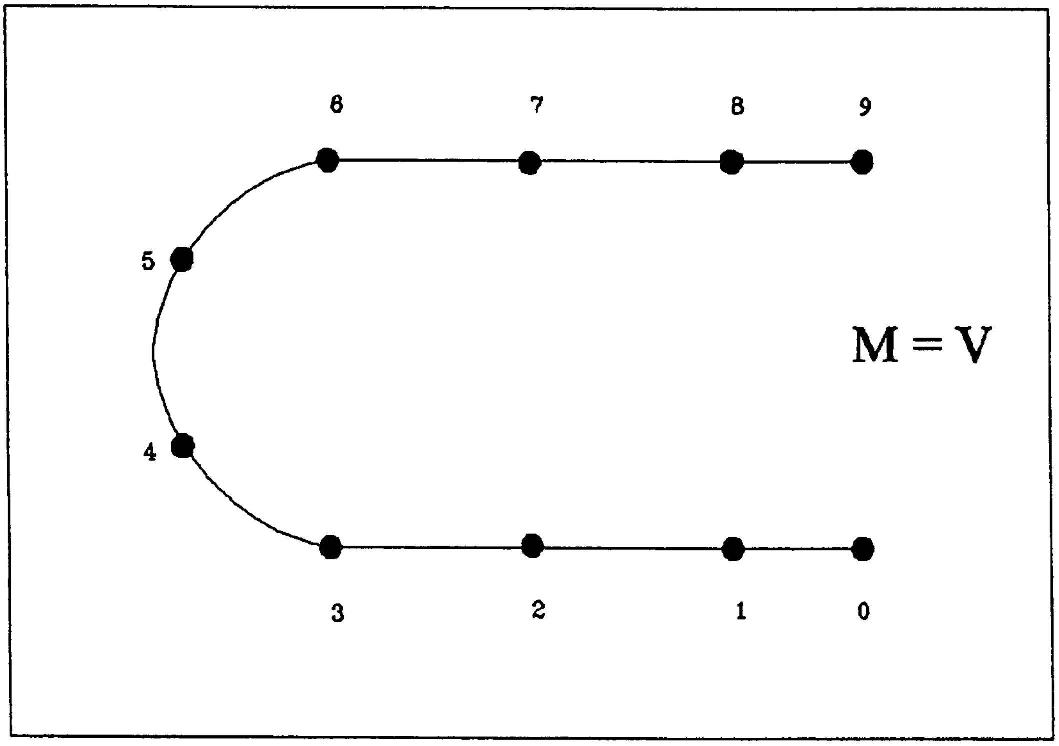

Figure 1: Example of a linear ($M = V$) data manifold together with the hypothetical positions of the images of the neural units.

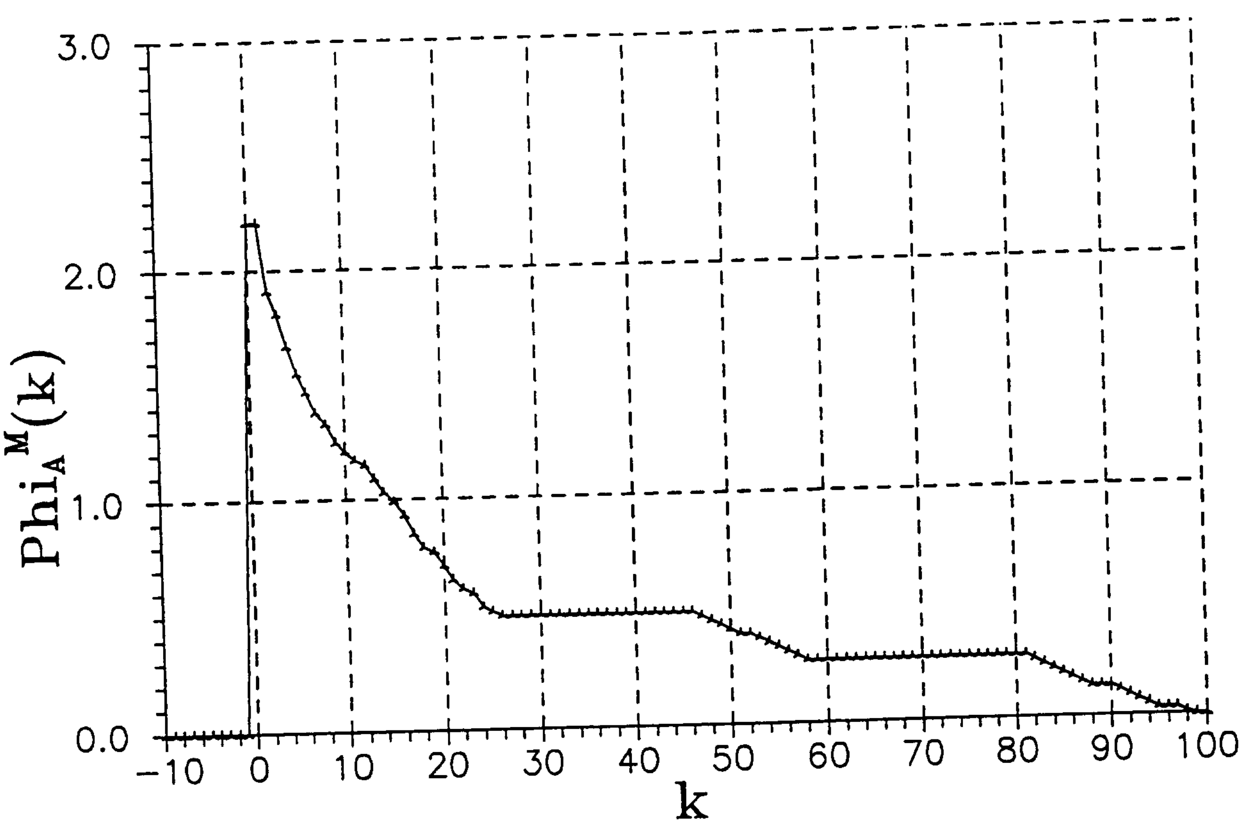

Figure 4: The topographic function of a map of a squared input space onto a chain of 100 neural units.

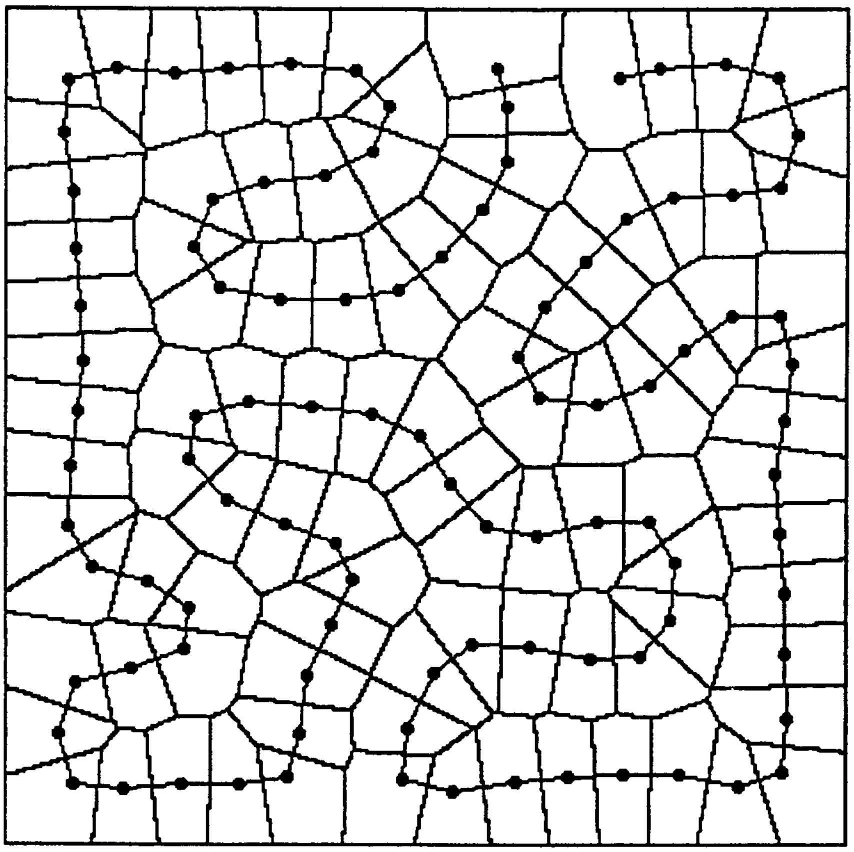

Figure 3: Plot of a map of a squared input space onto a chain of 100 neural units, the receptive fields of the units are shown.

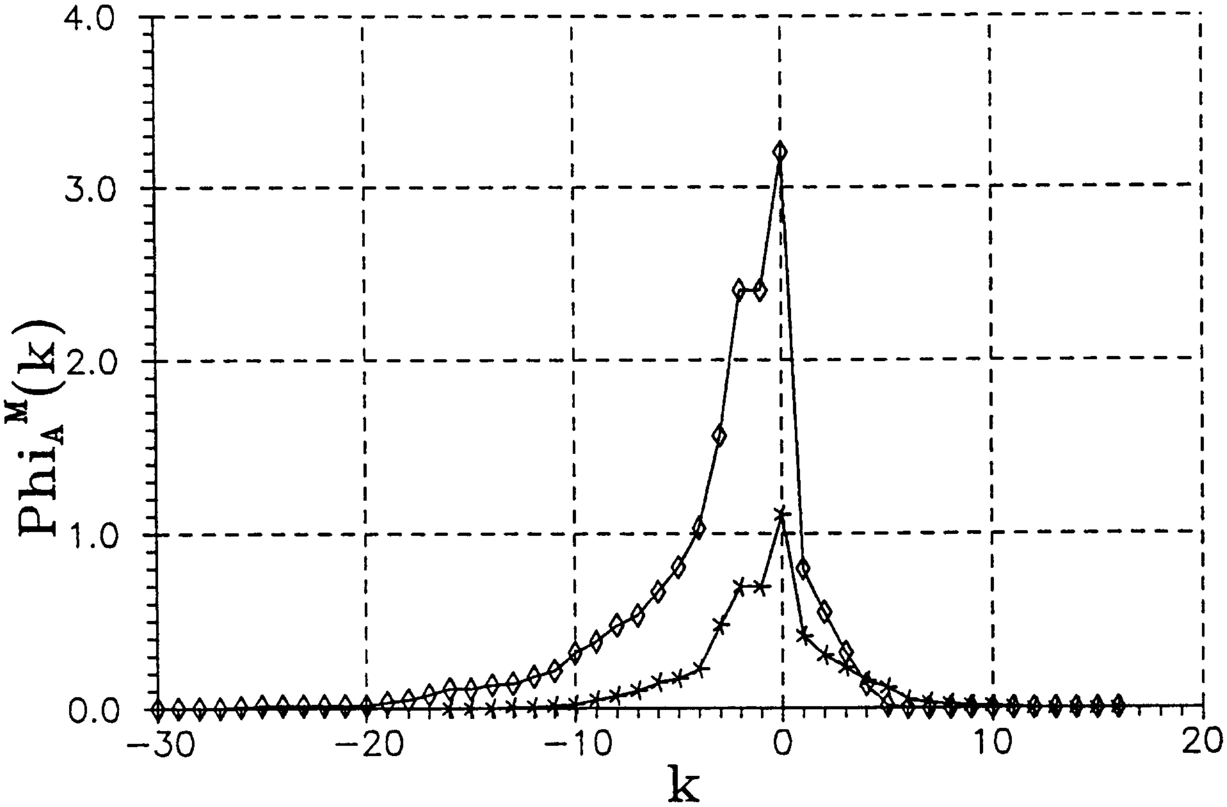

Figure 6: The topographic functions obtained from a map of a set of speech data onto a squared lattice of 16 × 16 neural units (points as ⋆) and onto a three-dimensional lattice of 7 × 6 × 6 neural units (points as ◇).

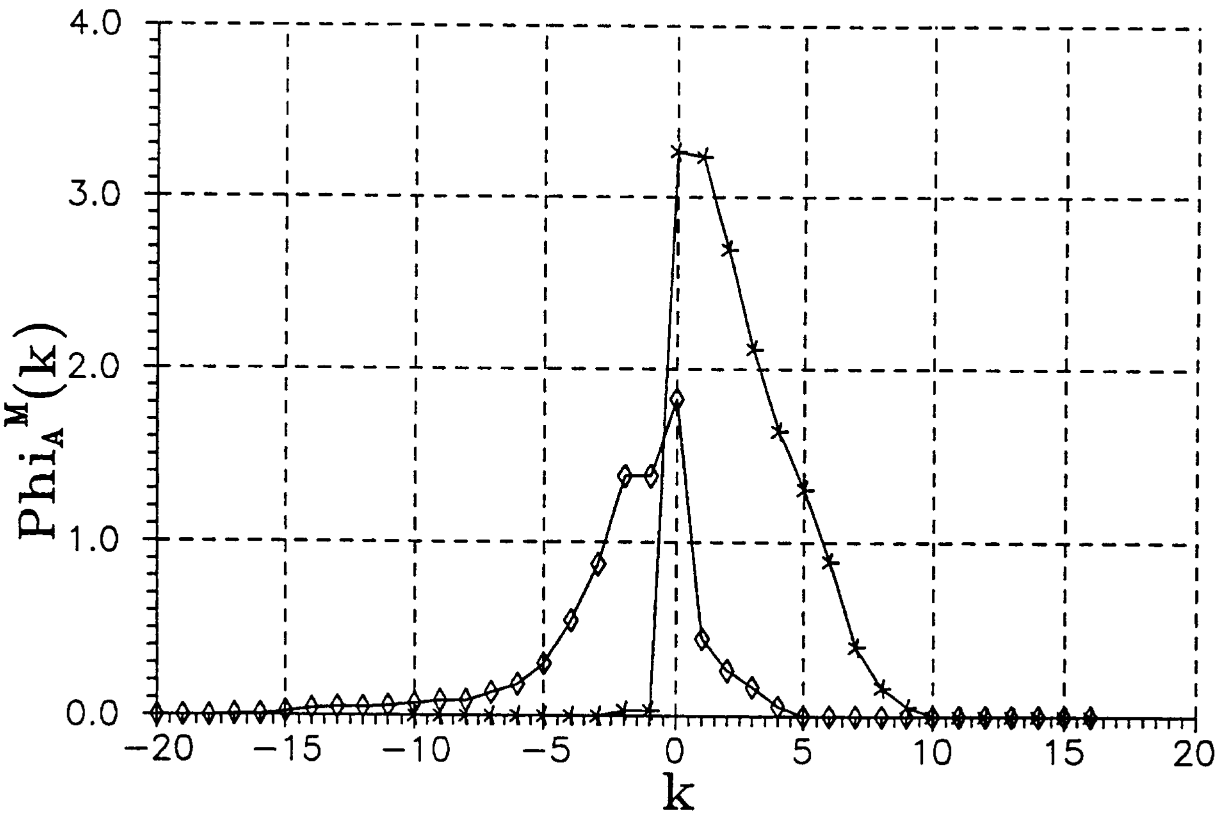

Figure 5: The topographic functions obtained from a map of a 6-dimensional LANDSAT TM satellite image onto a squared lattice of 16 × 16 neural units (points as ⋆) and onto a three-dimensional lattice of $7 \times 6 \times 6$ neural units (points as ◇).

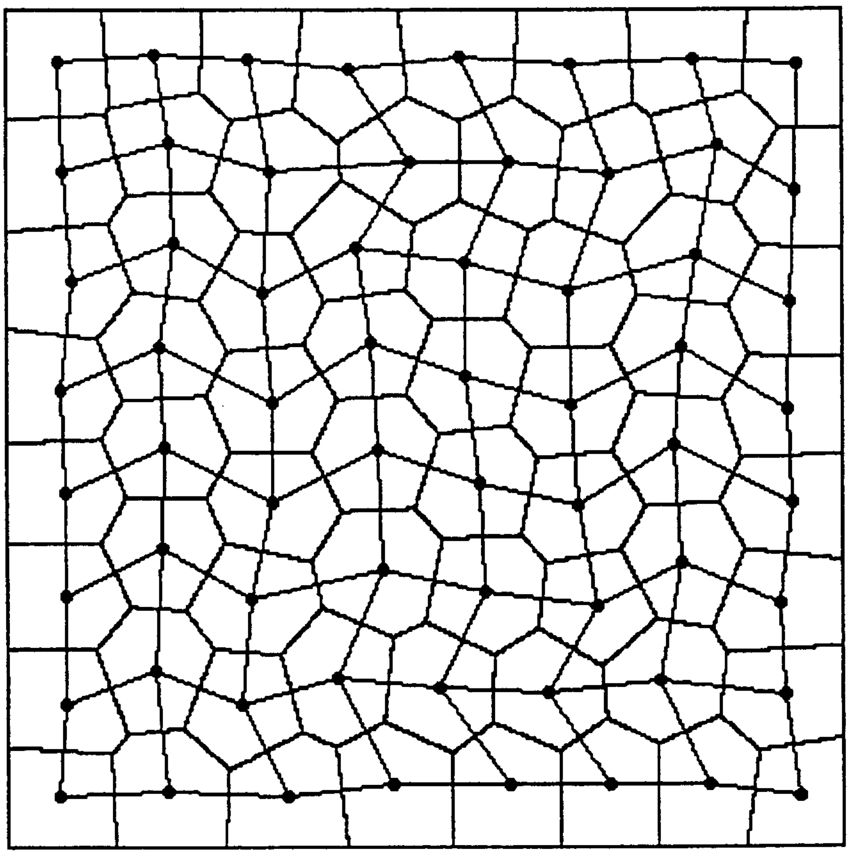

Figure 7: The receptive fields of a squared lattice of neural units.

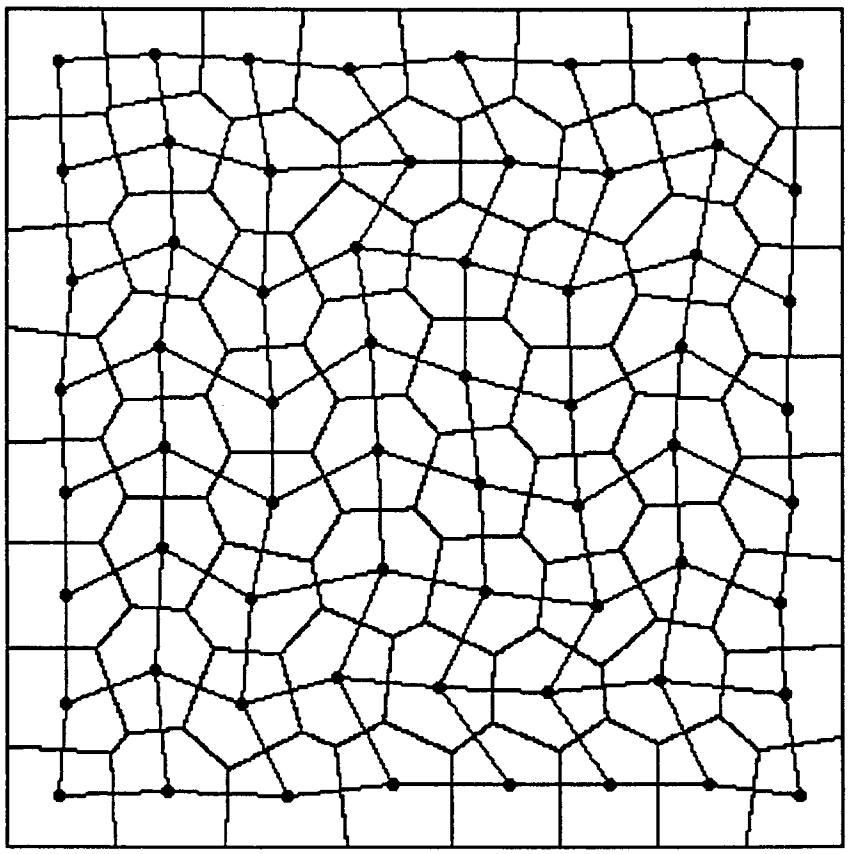

Figure 7: The receptive fields of a squared lattice of neural units.