Neural Networks 56 (2014) 35–48

Contents lists available at ScienceDirect

Neural Networks

journal homepage: www.elsevier.com/locate/neunet

Grid topologies for the self-organizing map

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HIGHLIGHTS

- The topologies of the map lattice for SOMs have rarely been researched.
- This work studies alternative map topologies to those used in previous literature.
- The theory of tessellations is used to obtain the alternative topologies.
- The alternative topologies outperform the classical ones in several tasks.
- A theory of SOFM topologies is developed.

ARTICLE INFO

Article history:
Received 5 February 2014
Received in revised form 28 April 2014
Accepted 1 May 2014
Available online 13 May 2014

Keywords:
Self-organizing map topologies
Tessellations
Clustering
Image segmentation
Classification

ABSTRACT

The original Self-Organizing Feature Map (SOFM) has been extended in many ways to suit different goals and application domains. However, the topologies of the map lattice that we can found in literature are nearly always square or, more rarely, hexagonal. In this paper we study alternative grid topologies, which are derived from the geometrical theory of tessellations. Experimental results are presented for unsupervised clustering, color image segmentation and classification tasks, which show that the differences among the topologies are statistically significant in most cases, and that the optimal topology depends on the problem at hand. A theoretical interpretation of these results is also developed.

1. Introduction

The proposal of the self-organizing map (Kohonen, 1990, 2001) has led to a vast body of knowledge, which includes many modifications and extensions of the original model (Kohonen, 2013). However, an aspect of the SOFM which has received little attention is the topology of the map lattice (Merkow & DeLisle, 2007). The standard choice is the square topology, with few exceptions which correspond to the hexagonal topology (Asgary, Naini, & Levy, 2012; Van Der Voort, Dougherty, & Watson, 1996). This observation poses two fundamental questions, which we aim to answer in this paper: (1) whether these two topologies have something that makes them special; (2) whether there are other topologies suitable for SOFMs.

It must be noted that there are many self-organizing models that do not consider a fixed grid topology, but a dynamic one which is learned from the data. These include the Growing Neural Gas (GNG) and the Growing Cell Structures (GCS), where the focus is on learning a topology that reflects the structure of the data by adding new neurons and connections in a controlled manner (Delgado, Gonzalo, Martinez, & Arquero, 2011; Fiser, Faigl, & Kulich, 2013; Forti & Foresti, 2006; Heinke & Hamker, 1998; Viejo, Garcia, Cazorla, Gil, & Johnsson, 2012). These are not considered self-organizing maps due to the absence of a lattice, so they are outside the scope of this paper. Their advantage is their flexibility to adapt to the input distribution. However they are less suitable for dimensionality reduction and visualization purposes, since in general terms the topologies that they generate cannot be projected on a plane without violating some neighborhood relations. This is because most graphs are not planar, i.e. they cannot be plotted on a plane without crossing connections. A model which stands between the GNG and the SOFM is the Evolving Self-Organizing Map (Deng & Kasabov, 2003). It considers a growing number of units and a dynamic neighborhood for each unit as the GNG does. On the other hand, the learning of the neighboring units is proportional to the topological connection strength and not to the rank in the list of neighbors, which is the strategy that the SOFM uses.

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http://dx.doi.org/10.1016/j.neunet.2014.05.001
0893-6080/

A second kind of models is based on grid topologies like the SOFM, but they allow the map to grow. Here the reference model is the Growing Hierarchical Self-Organizing Map, which builds a tree structure which grows horizontally and vertically according to a prespecified accuracy (Liu, Weisberg, & He, 2006; Lu & Wang, 2010; López-Rubio & Palomo, 2011; Rauber, Merkl, & Dittenbach, 2002). In this case we have a basic grid pattern which is repeated as the map is enlarged. Again, the standard choice is the square topology. Hence the alternatives that we present here can be applied to these models.

There is another line of research which calls for self-organizing networks with a growing number of units where the topology must fulfill some constraints even if it is not a fully regular grid. This strategy includes the Multilevel Interior Growing Self-Organizing Map (Ayadi, Hamdani, & Alimi, 2012), where the network must grow either from the boundary or from the interior of the current network topology, which is a multilevel 3D structure. The Cube Kohonen Self-Organizing Map model (Lim & Haron, 2013) is designed to represent 3D input distributions, and it aims to learn a correct wireframe topology for closed 3D surface data. Finally, the Cell Splitting Grid constrains the topology to lie on a square, so that a square cell is associated to each unit, and growth proceeds by splitting a square into four subsquares (Chow & Wu, 2004).

Other types of self-organizing networks include non growing tree structures such as the Self-Organizing Topological Tree (Xu, Chang, & Paplinski, 2005), which is particularly adequate for hierarchical input data and features a faster learning due to the tree nature of the network. Finally, the self-organizing graphs (López-Rubio, Muñoz-Pérez, & Gómez-Ruiz, 2002; López-Rubio, Palomo-Ferrer, Ortiz-de Lazcano-Lobato, & Vargas-González, 2011), feature dynamic connections which are learned while the number of neurons is kept fixed. This way the adaptation to the structure of the input is not done at the expense of enlarging the network. This is desirable because there must be a balance between the complexity of the model (number of neurons) and its accuracy when representing the input data (vector quantization error). Moreover, in some applications a codebook with a fixed length is needed (for example, to fit a code with a specified number of bits), so a constant number of neurons is required.

From the preceding it can be concluded that many ways of learning topologies have been developed for self-organizing networks, but fixed grid topologies have not been explored adequately. Our aim here is to propose grid topologies for the SOFM which offer good performance in terms of vector quantization and topographic quality.

The structure of this paper is as follows. First some fundamental concepts are reviewed; they will be used through the paper (Section 2). Then the alternative topologies for self-organizing maps are presented and compared from a theoretical viewpoint (Section 3). Experiments with real data are shown in Section 4. Some important properties of the proposal are discussed in Section 5, and possible answers for the two fundamental questions posed before are given. Finally, Section 6 is devoted to conclusions.

2. Basic concepts

In this section the fundamental concepts which this work is based on are reviewed. First a brief outline of Kohonen's Self-Organizing Feature Map (SOFM, Kohonen (1990)) is presented, leaving the grid topology unspecified (Section 2.1). Then we discuss the types of tilings of the plane (Section 2.2). The grid topologies that we propose in Section 3 are chosen from them.

2.1. Review of the self-organizing map

Next we are going to review the original Kohonen's SOFM to present the notation that will be used through the paper. Let M be the number of neurons of the self-organizing map, which are arranged in a lattice of size $a \times b$, where $M = ab$. The topological distance between the neurons i and j, located at positions $\mathbf{r}_i, \mathbf{r}_j \in \mathbb{R}^2$ in the lattice plane, is given by:

$$d(i, j) = \left\| \mathbf{r}_i - \mathbf{r}_j \right\|. \tag{1}$$

Every neuron i has a prototype vector $\mathbf{w}_i$ which represents a cluster of input samples. Please note that $\mathbf{w}_i \in \mathbb{R}^D$, where D is the dimension of the input space. At time step n, a new sample $\mathbf{x}(n)$ is presented to the network, and a winner neuron is declared:

$$Winner(\mathbf{x}(n)) = \arg \min_{j \in \{1,\dots,M\}} \left\| \mathbf{x}(n) - \mathbf{w}_j(n) \right\|. \tag{2}$$

Then the prototypes of all the units are adjusted, for $i \in \{1, \dots, M\}$:

$$\begin{aligned} &\mathbf{w}_i(n+1) \\ &\quad = \mathbf{w}_i(n) + \eta(n)\, \Lambda(i, Winner(\mathbf{x}(n)))\, (\mathbf{x}(n) - \mathbf{w}_i(n)) \end{aligned} \tag{3}$$

where $\eta(n)$ is a decaying learning rate and the neighborhood function Λ varies with the time step n and depends on a decaying *neighborhood radius* $\Delta(n)$:

$$\eta(n+1) \le \eta(n) \tag{4}$$

$$\Lambda(i, Winner(\mathbf{x}(n))) = \exp\left(-\left(\frac{d(i, Winner(\mathbf{x}(n)))}{\Delta(n)} \right)^2 \right) \tag{5}$$

$$\Delta(n+1) \le \Delta(n). \tag{6}$$

The receptive field of neuron i, i.e. the region of the input space which is represented by i, is defined as:

$$F_i = \left\{ \mathbf{x} \in \mathbb{R}^D \mid i = Winner(\mathbf{x}) \right\}. \tag{7}$$

2.2. Tilings of the plane

There are many possible tilings of the plane. Aperiodic (non repetitive) and even fractal tilings are of great importance to science and engineering (Cervelle & Durand, 2004; Currie & Simpson, 2002; Morabito, Isernia, Labate, D'Urso, & Bucci, 2009; Ostromoukhov, 2007; Palagallo & Salcedo, 2008). However, for our purposes only periodic tilings are useful, since we want the maps to have the same topological structure at every location. Moreover, we restrict our attention to edge-to-edge tilings, i.e. if two polygons intersect at more than one point, then they share a whole edge (Chavey, 1989). This is because non edge-to-edge tilings lead to neurons with only two neighbor neurons, since a neuron is to be placed at every vertex of each polygon. Such an arrangement could lead to poor cooperation among neurons due to the sparse connectivity. The type of a vertex is a listing of the numbers of edges of the polygons that meet the vertex, separated by dots. Superindices are used to note runs of the same kind of polygon. As usual in tessellation theory, we name tilings by their vertex types (Grünbaum & Shephard, 1987).

The elements of a tiling are the tiles, the edges and the vertices. The equivalence classes of the elements of a tiling under its symmetry group are called orbits. This means that if two elements are in the same orbit, then we can carry one into the other by a symmetry of the tiling. Since the neurons of the map are associated with the vertices, a tiling with only one vertex orbit generates a map where all the neurons are symmetric with each other. This is a nice property for a self-organizing map, so we impose this condition too.