Effects of Irregular Topology in Non-Planar SOM Variants

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1 Background and Lit Review

The Self-Organizing Map (SOM) is an unsupervised competitive learning process developed by Teuvo Kohonen as a technique to analyze high dimensional data sets. The SOM algorithum uses an artificial neural network to organize high dimensional data onto a low dimensional lattice, or map, of neurons. Each neuron contains a reference vector that can be considered to model a portion of the input space. Before training these neurons are initialized, most commonly to random values. During the training process a randomly selected input vector searches the map for its best matching unit (BMU), that is the neuron to which it is most similar. The BMU and its neighborhood, as defined by a neighborhood function, are than adjusted to better match that observation (Kohonen, 2000). The training process is repeated a predefined number of times, or ideally until the map converges. The traditional SOM is laid out on a two dimensional plane using either a rectangular or hexagonal topology. According to Wu and Takatsuka (2006) the hexagonal structure is more uniform and generally preferred.

One obvious drawback of building the neural lattice in a discrete euclidean plane is the boundary of the resulting lattice. A neuron located on the boundry has fewer neighbors and thus fewer chances of being updated (Wu and Takatsuka, 2006). As observed in Figure 1, neurons in the center of the map tend to better represent the mean of the input-space. This is arguably caused by outliers being pushed to the edges of the map, where they encounter fewer competing signals.

1.1 Spherical SOM

A natural way to eliminate the boundary effect is to wrap the lattice around a three dimensional object such as a sphere or torus, therefor removing the edge entirely. The toroidal SOM was introduced by Li et al. (1993), however the torus is not hugely effective for visualization, as maps generated from a torus are not very intuitive (Ito et al., 2000; Wu and Takatsuka, 2006). Ritter (1999) describes the torus as being topologically flat and suggests that a curved topology, such as that of a sphere, may better reflect directional data. A sphere also results in a more intuitive map, since we are accustomed to looking at maps based on a sphere.

Ritter (1999) first introduced the spherical SOM and several enhancements have since been suggested (Boudjemai et al., 2003; Sangole and Knopf, 2003; Nishio et al., 2006; Wu and Takatsuka, 2006). A good comparison of these enhancements can be found in (Wu and Takatsuka, 2006). All of these methods derive their spherical structure through the tessellation of a polyhedron as

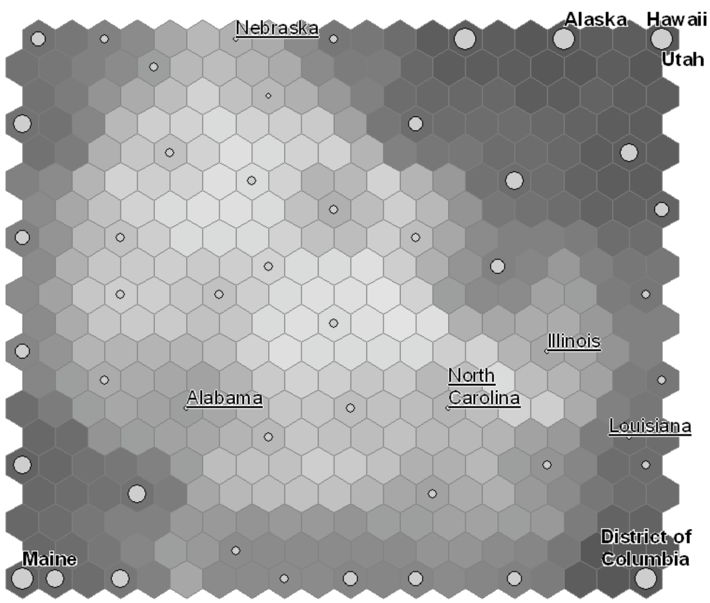

Figure 1: Fifty states plus D.C. mapped onto SOM trained with the first thirty-two census variables. Darker neurons have a relatively large differences from the mean of the states, while lighter neurons are relatively closer. Larger dots represent inputs that were poorly fit to the map, small smaller dots show inputs that were better bit to the map.

originally proposed by Ritter. Wu and Takatsuka (2006) point out the importance of a uniform distribution on the sphere and that it is preferable for all neurons to have an equal number of neighbors and to be equally spaced. They find generally that the tessellation method best satisfies these conditions and specifically that the icosahedron is the best starting point (Wu and Takatsuka, 2005). Tessellation of the icosahedron results in a network of neurons, each of which have exactly six neighbors, save the original twelve which each have five. This is very close to the ideal structure in which every neuron would have exactly six neighbors. This structure has very low variances in both neuron spacing and neighbor size.

1.2 Network Size

The cost of releying on Ritter's tesselation method is decreased control over network size. Ritter's tesselation methods results in a rework site that grows at a rate of $N = 2 + 10 * 4^f$. Wu and Takatsuka (2006) offer a slight improvement, rather then recursivly subsidiveding the faces, they redivid the original icosehdron with each step resulting in $N = 2 + 10 * f^2$.

The tessellation method used by the class of spherical SOMs based on Ritter's work results in a network size that is a function of the tessellation frequency and therefore grows exponentially. In practice 2D Euclidean SOMs also offer limited control over network size, as it is undesirable to have one dimension dramatically larger then the other. Nishio et al. (2006) try to address the issue of network size granularity by departing from the tessellation method and suggesting the use of a partitioned helix to uniformly distribute any number of neurons on a sphere. A similar method was dismissed by Wu and Takatsuka (2005) for failing to satisfy the uniformity conditions. Nishio et al. seem to have addressed variance in nearest neighbor distances, but the issue of having a uniform number of direct neighbors is still not addressed.

The literature offers little theoretical guidance on network size (Cho et al., 1996). Vesanto (2005) suggests simply using a network size of $5 * \sqrt{n}$, where n is the number of observations.

1.3 Uniformity

Wu and Takatsuka state that "[f]or SOM, it is desirable to have all neurons receive equal geometrical treatment" (Wu and Takatsuka, 2006, pp. 900). To satisfy this constraint two conditions must be met. Firstly, each neuron should occupy the same amount of space on the given surface. Secondly, each neuron should be bordered by the same number of surrounding neurons, and we should maximize that number. The first condition in hugely important for visualization, but irrelevant for training. During the training of the SOM only the topology of the neurons is considered.

Based solely on measures of neuron spacing Wu and Takatsuka (2005) dismissed a method proposed by Rakhmanov et al. (1994) for distributing points on a sphere. Similarly Nishio et al. (2006) use these variance measures to support their helix algorithm for distributing points on a sphere. Table 1 shows that these metrics can be misleading and may not be comparable across topologies. The traditional rectangular and hexagonal topologies have no variance in neuron spacing and the generally preferred hexagonal structure displays greater variance in neighborhood size than the rectangular structure. The torus by comparison would have variance in neuron spacing, yet no variance in neighborhood size. The distance between two neurons is only considered during the formation of the neuronal network. At this stage the spacing is significant as it plays a part in determining neuron adjacency. However using this measure to evaluate potential topologies for use in SOM may be misleading.

Table 1: Variances in Topologies

Topology	Grid Size	Neuron Spacing	Variance in Neighborhood Size
Rectangular	9x18	1	0.2716
Hexagonal	9x18	1	1.2138
Tessellation	162	0.25319 - 0.31287	0.0686
Rakhmanov	162	0.15779 - 0.30069	0.2908

Methods, for distributing points on the sphere, which allow for fine grained control over network size produce slightly more irregular topologies. However, no discussion of these irregularities or their effects on SOM training has occurred in the literature. Given that limited theoretical guidance is available for choosing network size the desire for finer control over the network size, should not be overlooked. In particular for a larger SOM the ideal network size may not be achievable via tessellation of the icosahedron.

2 Data and Methodology

It is useful to represent our neural lattice as a graph, G. We know that any arrangement of neurons onto the surface of a sphere will as such the network can be effectively treated as a graph. Doing so enables us to use the properties of the graph and the principles of graph theory to help us understand the relationship between neurons during training.

the variance in neuron spacing should be minimized. The first condition ensures that each neuron will occupy is only of concern when visualizing the SOM.

The get at the second condition we must first define the degree of a neuron, deg(n) to be number of its direct neighbors. Whit that in mind the second condition is that the variance in the degree of the neurons must also be minimized.

This statement may be somewhat misleading to those investigating alternative

For the purpose of SOM visualization it is important for each neuron to receive equal geometrical treatment.

It is useful to represent the neural network as a graph, G, in order use the... In order to examine the irregularites in the neural network it is useful ....

The basic problem of the "boundary effect" is that neurons on the edge have fewer neighbors. Yet there are only five possible arrangements of points on a sphere such that all points have the same number of neighbors. Any spherical lattice consisting of more then twenty (dodecahedron) neurons will contain topological irregularities. This is to say that not all neurons will have the same number of neighbors. The importance of these irregularities and the magnitude of their effects on SOM training is not known. This goal of this research is to determine whether more flexible network structures may be used in spherical in SOM without introducing significant errors. To accomplish this goal, basic methods in network analysis with be combined with the result from several empirical training runs each utilized different topology.

2.1 Synthetic Data

In order to have a basis for comparison

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