

The self-organizing map, the Geo-SOM, and relevant variants for geosciences

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Received 1 July 2003; received in revised form 1 June 2004; accepted 1 June 2004

Abstract

In this paper we explore the advantages of using Self-Organized Maps (SOMs) when dealing with geo-referenced data. The standard SOM algorithm is presented, together with variants which are relevant in the context of the analysis of geo-referenced data. We present a new SOM architecture, the Geo-SOM, which was especially designed to take into account spatial dependency. The strengths and weaknesses of the different variants proposed are shown through a set of tests based on artificial data. A real world application of these techniques is given through the analysis of geodemographic data from Lisbon's metropolitan area.

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Keywords: Self-Organizing Map; Geo-SOM; SOM variants; Geo-referenced data

1. Introduction

The sophistication of today's geo-referenced data collection technologies has created a continuous stream of data which has been flooding our databases. This trend will build up in the next years as already available technologies find their way into our daily lives. Data collection through location-aware devices, high-resolution remote sensing systems, decennial census operations and the storing and management capabilities of Geographic Information Systems (GIS) made available colossal volumes of geo-referenced data. This fact created opportunities for developing an improved understanding of a number of environmental and socio-economic phenomena that are at the heart of GIScience (Openshaw, 1999). Nevertheless, it also shaped new challenges and difficulties on the analysis

of multidimensional geo-referenced data. Today, the availability of methods able to perform intelligent reduction, on huge amounts of high-dimensional geo-referenced data, is a central issue in GIScience.

The need to transform into knowledge the massive digital geo-referenced databases has led geoscientists to search for new tools, tools that are able to tame complexity. The field of knowledge discovery constitutes one of the most relevant stakes in GIScience research to deal with this problem (Gahegan, 2003, Miller and Han, 2001). Although knowledge discovery and data mining have put forward numerous methodologies and tools, the need to adequate those tools to the specific context of GIScience remains a research challenge for geoscientists (Openshaw, 1999).

More than prediction tools we need to develop exploratory tools based on classification and clustering which enable an improved understanding of the available data. It has been suggested that neurocomputing paradigms, such as the Self-Organizing Map (SOM)

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(Openshaw et al., 1995, Openshaw and Wymer, 1995), may provide the power and flexibility to improve the overall quality of multidimensional geo-referenced data classifications. The combination of better classification algorithms and explicit focus on the issues of geographic representation will certainly reap sizeable rewards. The challenge is to be able to incorporate geo-reasoning into the existing tools.

In this paper we concentrate on the application of the SOM in the reduction of large volumes of multi-dimensional geo-referenced data. More specifically, we are interested in looking at the possibility of introducing geographical knowledge within the classification process. In order to test proposed variants of the SOM, two artificial data sets and a census database of the metropolitan area of Lisbon are used.

We propose three different variants of the SOM which enable the explicit incorporation of geographic space within the workings of the SOM algorithm, and experimentally evaluate one of them. More specifically, we try to explore the flexibility of the SOM to develop approaches that can improve the existing classification methods of multidimensional geo-referenced data.

In the next section an explanation of the workings of SOM is given, along with a more detailed explanation of the variants proposed. After that we perform some tests on the artificial data sets. Next we present the main results of the application of one of the variants to the Lisbon metropolitan area data. Finally, some conclusions are drawn.

2. Self-Organizing Map

Although the term “Self-Organizing Map” could be applied to a number of different approaches, we shall use it as a synonym of Kohonen’s self-organizing map, or SOM for short. These maps are also referred to as “Kohonen neural networks” (Fu, 1994), “self-organizing feature maps—SOFM”, “topology preserving feature maps” (Kohonen, 1995), or some variant of these names. Kohonen describes SOM as a “visualization and analysis tool for high-dimensional data”, but they have been used for clustering (Vesanto and Alhoniemi, 2000), dimensionality reduction, classification, sampling, vector quantization, and data mining (Kohonen, 2001).

The basic idea of a SOM is to map the data patterns onto an n -dimensional grid of neurons or units. That grid forms what is known as the output space, as opposed to the input space that is the original space where the data patterns are. This mapping tries to preserve topological relations, i.e. patterns that are close in the input space will be mapped to units that are close in the output space, and vice versa. The output space will usually be two-dimensional, and most of the

implementations of SOM use a rectangular grid of units. So as to provide even distances between the units in the output space, hexagonal grids are sometimes used (Kohonen et al., 1995). Single-dimensional SOMs are common, e.g. for solving the travelling salesman problem (Maenou et al., 1997), and some authors have used three-dimensional SOMs (Takatsuka, 2001). Using higher-dimensional SOMs (Villmann et al., 2003), although posing no theoretical obstacle, is rare, since it is not possible to easily visualize the output space.

Each unit, being an input layer unit, has as many weights or coefficients as the input patterns, and can thus be regarded as a vector in the same space as the patterns. When we train or use a SOM with a given input pattern, we calculate the distance between that pattern and every unit in the network. We then select the unit that is closest to the winning unit (best matching unit—BMU), and say that the pattern is mapped onto that unit. If the SOM has been trained successfully, then patterns that are close in the input space will be mapped to neurons that are close (or the same) in the output space, and vice versa. Thus, SOM is “topology preserving” in the sense that (as far as possible) neighbourhoods are preserved through the mapping process.

Before training, the neurons may be initialized randomly. During the first part of training, they are “spread out”, and pulled towards the general area (in the input space) where they will stay. This is usually called the unfolding phase of training. After this phase, the general shape of the network in the input space is defined, and we can then proceed to the fine tuning phase, where we will match the neurons as far as possible to the input patterns, thus decreasing the quantization error.

The basic SOM learning algorithm may be described as follows:

Let

w_{ij} be the weight vector associated with unit positioned at column i row j

x_k be the vector associated with pattern k

d_{ij} be the distance between weight vector w_{ij} and a given pattern.

h be a neighborhood function described below.

α be the learning rate also described below.

For each input pattern:

- (1) Calculate the distance between the pattern and all units of the SOM ($d_{ij} = ||x_k - w_{ij}||$) (this is called the calculation phase)
- (2) Select the nearest unit as winner w_{winner} ($w_{ij} : d_{ij} = \min(d_{mn})$) (this is what is usually called the voting phase)

- (3) Update each unit of the SOM according to the update function $w_{ij} = w_{ij} + \alpha h(w_{winner, w_{ij}} || x_k - w_{ij} ||)$ (this is what is usually called the updating phase)
- (4) Repeat the steps (1) to (3), and update the learning parameters, until a certain stopping criterion is met.

This algorithm can be applied to a SOM with any dimension. The learning rate α , sometimes referred to as η , varies in the $[0,1]$ interval and must converge to 0 so as to guarantee convergence and stability for the SOM. The decrease from the initial value of this parameter to 0 is usually done linearly, but any other function may be used.

The radius, usually denoted by r , indicates the size of the neighbourhood around the winner unit in which the units will be updated. This parameter is particularly relevant as it defines the topology of the SOM, deeply affecting the unfolding of the output space. Initially, r can be as big as the size of the network, but in order to guarantee convergence and stability it has to converge to 1 or 0. For the sake of simplicity, r is sometimes omitted as an explicit parameter. The update of both α and r may be done after each training pattern is processed or after the whole training set is processed.

The neighbourhood function h , sometimes referred to as A or N_c , assumes values in $[0,1]$, and is a function of the position of two units (a winner unit and another unit), and radius, r . It is large for units that are close in the output space, and small (or 0) for units far away. Usually, it is a function that has a maximum at the centre, monotonically decreases up to a radius r and is zero from there onwards. The two most common neighbourhood functions are the bell-shaped (Gaussian-like) and the square (or bubble).

To visualize the results of a SOM, U-matrices (Ultsch and Siemon, 1990) may be used. The U-matrix is a representation of a SOM in which distances, in the input space, between neighbouring neurons are represented, usually using a colour or grey scale. If distances between neighbouring neurons are small, then these neurons represent a cluster of patterns with similar characteristics. If the neurons are far apart, then they are located in a zone of the input space that has few patterns, and can be seen as a separation between clusters. The U-matrix constitutes a particularly useful tool to analyze the results of a SOM, as it allows an appropriate interpretation of the clusters available in the data.

3. SOM variants

A very large number of SOM variants have been proposed, and reviews of some of these can be found in Kangas et al. (1990), Kaski (1997), Kohonen (2001), and

Vesanto and Alhoniemi (2000), but little work has been done in the context of adapting the SOM to the specific problems and paradigms of geosciences. Some of the variants that can be found are just parameterizations or minor adjustments to the basic SOM algorithm, while others differ quite a lot and do not have the same mapping and visualization properties of the SOM. We shall now review some of the major variants which we consider to be relevant in geo-referenced data analysis, and present ways in which they may be applied.

3.1. Geo-enforced SOM

One simple way to modify the SOM and make it more adequate to process geo-referenced data is based on producing quasi-variants and testing spatial effects is through the use of pre-processing. The Geo-enforced quasi-variant is based on weighting the geographic coordinates in order to make them as important as all other variables available. This way each geographic coordinate is multiplied by a constant, thus attributing the same importance to the two geographical variables as the rest of the entire set of variables. The weight that should be attributed to the geographic coordinates is defined by the user. Although subjective the decision will determine the type of results achieved. Apart from the subjectivity associated with the weighting of the geographic variables, there is an additional problem in this approach. Geographical locations that are located far apart from the centre of the geographic distribution will always be deficiently represented.

3.2. Hierarchical SOMs

Hierarchical SOMs are often used in application fields where a structured decomposition into smaller and layered problems is convenient. One or more than one SOMs are located at each layer, usually operating on different thematic variables (see Fig. 1).

The hierarchical SOMs were first introduced in Ichiki et al. (1991), and were extensively used in speech recognition, where each layer deals with higher units of speech, such as phonemes, syllables and word parts

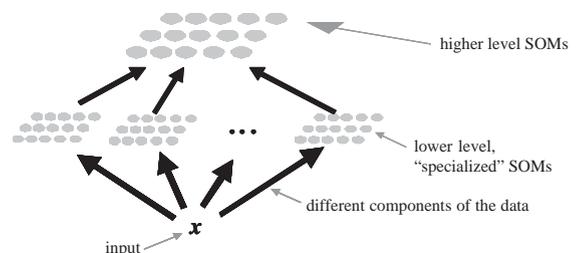


Fig. 1. Structure of a hierarchical SOM.

(Behme et al., 1993; Kemke and Wichert, 1993; Jiang et al., 1994).

Hierarchical SOMs can have several lower level partial maps that cluster the data according to different characteristics and then pass the results to an upper level SOM, or they may have a lower level global SOM, that acts as a gating mechanism to activate one of several higher level SOMs that specialize in a certain area of the input space.

In terms of geosciences one can envision the usefulness of hierarchical SOM in applications like geodemographics. The hierarchical SOM allows the creation of purpose-specific or thematic classifications at lower layers which are then composed into a single one. This can constitute a major advantage as it has been noted that the single-purpose geodemographic classifications constitute more powerful tools than general-purpose classifications (Openshaw and Wymer, 1995). Additionally, the exploration of the different SOMs at lower levels can be very valuable, especially if done in a computational environment where dynamic linking between SOMs can be set up. This way the interactive exploration of the different classifications can provide major insights. The idea is to take one of the SOMs, select specific units and study the distribution of the input patterns classified in that particular unit in the other SOMs and in the geographic space.

3.3. Geo-SOM

Another way of incorporating some geographical reasoning is to introduce the first law of geography (Tobler, 1970) in the training of a SOM. This would suggest that when seeking the winning unit for a certain data pattern, only the neurons geographically close to the data pattern should be searched. Just how close the candidates for BMU should be can be defined by a variable k , which we call “geographical tolerance”. If we make this geographical tolerance $k = 0$, then we force the BMU to be the unit that is geographically closest. Increasing k allows units that are within a radius k (measured in the output space) to be potential BMUs. If k is of the order of the size of the map, then it has no influence in the search for BMU and we have the standard SOM. This approach has similarities with the Hypermap approach (Kohonen, 1991), where only part of the input features are used to find the best match, and with the Kangas architecture (Kangas, 1992), where only a small number of neighbours, in the output space of the previous winner, are searched. More generally, it is the idea of selecting only a subset of neurons as candidates for the winning unit that leads to what we call a Geo-SOM (see Fig. 2).

In this architecture the selection of the best match unit, or winning unit, is done in two steps. First, a best match is searched using only the geographical coordi-

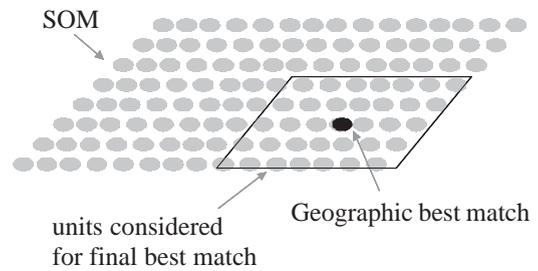


Fig. 2. Structure of a Geo-SOM.

nates of the input vector. Only the units in the output space neighbourhood of this first best match are then compared to the complete input pattern, to select the final best match. The units are then updated according to the standard rule. The Geo-SOM forces units that are close in the output space to be close in the input space too, thus creating clusters of areas that will be geographically close.

4. Experiments with artificial data

In order to assist the comprehension of the major characteristics and properties of the different SOM variants presented, a set of tests based on artificial data is carried out. The objective of using artificial data is to produce a controlled environment where certain features of the variants can easily be understood. Next we present two experiments in which different SOM variants were tested, with particular emphasis on the Geo-SOM.

4.1. Experiment 1

For this example we used a set of 200 data points evenly spaced on a surface with coordinates $x \in [0,1]$, $y \in [0,2]$. Each point is associated with a single feature z which is 0 whenever $0.5 < y < 1.5$, and 10 otherwise, as can be seen in Fig. 3.

If we cluster the data based on non-geographical features, then we will have two very well defined clusters: one where $z = 10$ and another where $z = 0$, as can be seen in Fig. 4. If we consider only geographical coordinates, then we will have no well-defined clusters, since the points are evenly spaced. If we consider all three components, we may or may not obtain well-defined clusters. If no pre-processing is done, and since in this case the geographical feature has a very small scale when compared to the other feature, we will basically obtain only two clusters. If we pre-process the data points to have approximately the same scale in all components, we will obtain rather fuzzy clusters. Depending on the different scalings, we may obtain 1,

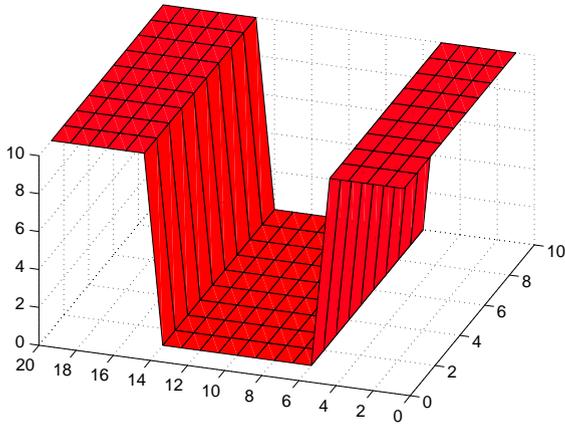


Fig. 3. Artificial data for experiment 1.

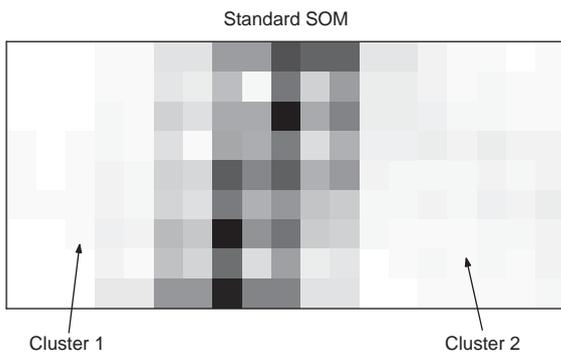


Fig. 4. U-matrix obtained using a standard SOM on artificial data of experiment 1.

2 or 3 clusters, but never clear-cut separations. A Geo-SOM with 0 tolerance will simply calculate local averages, and thus will just smooth the original data set, and the three clusters will still appear clearly in the U-matrix. The best results are obtained using a Geo-SOM with $k = 2$, as can be seen in Fig. 5. It is interesting to note that a 0 tolerance in the Geo-SOM produces blurred clusters, while relaxing this constraint will allow the clusters to define themselves better without losing their geographic localization.

4.2. Experiment 2

We constructed a second toy problem, this time comprising 5000 data points, each of which has geographical coordinates (x and y), and a third variable z that represents non-geographical data. The points follow a uniform distribution in the geographical coordinate, within the rectangle limited by $[(0,0), (20, 5)]$ (see Fig. 6). In the non-geographical dimension there are three zones of high spatial autocorrelation, where the values of z are very similar among neighbouring

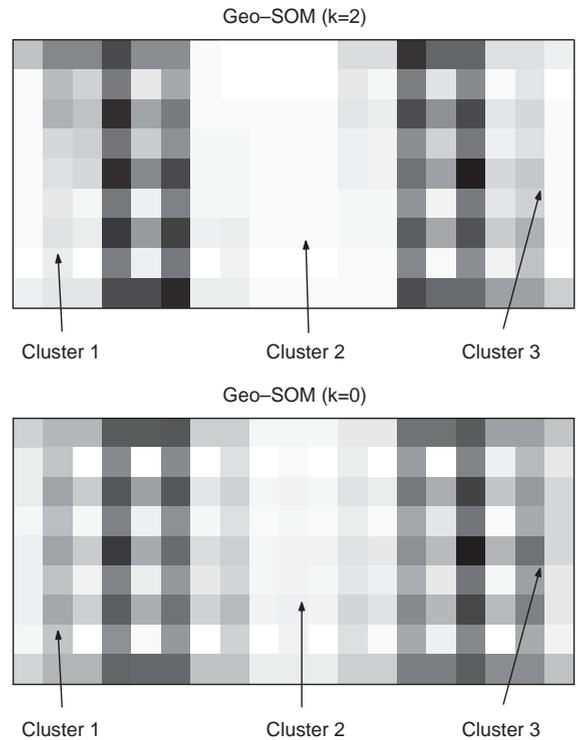


Fig. 5. U-matrices obtained using Geo-SOMs on the artificial data of experiment 1.

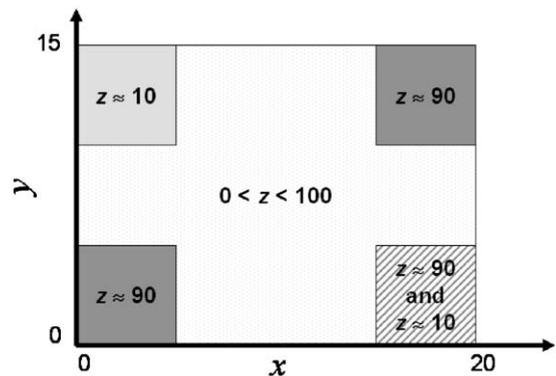


Fig. 6. Artificial data for experiment 2.

points, with a uniform in $[90, 91]$ in two zones and $[10,11]$ in another. There is also one area of “negative autocorrelation”, where half the data points have $z \approx 10$ and the other half have $z \approx 90$. In the rest of the input space z has a uniform distribution in $[0,100]$.

Here we compare a standard SOM with the Geo-SOM. In order to get a clear image of the error produced by each one of the tested variants, we decided to separate the error in geographic error and quantization error. The geographic error computes the average

distance between each input pattern and the unit to which it was mapped. This gives a notion of the geographic displacement of the units relative to the input patterns they represent. The quantization error provides an assessment of the distances between input patterns and the unit to which they are mapped in the attribute space, in this case the z variable. The quantization error provides a measure of the quality of the representation of z (non-geographical attributes) achieved.

The results are quite elucidative in the sense that they allow a very clear distinction between the behaviours of the different variants. Clearly, the restrictions imposed by Geo-SOM tend to degrade the quantization error and improve the geographic error. In terms of quantization error the highest value is observed, as would be expected, in the Geo-SOM. The actual values may be seen in Table 1.

The quantization errors shown in the table are averages for all data patterns, and the individual values vary quite a lot. A close inspection of the way this quantization varies allows us to identify different clusters, which is one of the main purposes of using these techniques. If we calculate the average quantization error of the input patterns that are mapped to each individual unit and plot these values in a contour plot, we obtain the results presented in Fig. 7. In this figure we plot the quantization error as a function of the geographical coordinates when using the Geo-SOM and the standard SOM.

The Geo-SOM provides interesting insights into the data. Homogeneous areas are very evident, as areas with low quantization error appear throughout the map. The lower right corner, where the data follow two distinct behaviours, is divided (approximately along its diagonal) into two homogeneous areas, one containing each type of data. These are separated by another area that serves as border, where the quantization error is quite large. A careful inspection of the remaining area shows stripes of low quantization error. These areas of low quantization are in general surrounded by sharp frontiers, which can be easily identified by the presence of smaller than average Thiessen polygons. As a conclusion, this map allows us to gain insight into less well structured areas of the data.

When using the standard SOM, the map has little information about the geographical organization of clusters. Since these are defined mostly by non-geographical attributes, their geographical location is basically meaningless and may lead to errors. The lower left

Table 1
Average geographical and quantization errors for artificial data of experiment 2

Type of map vs. type of error	Geo-SOM	Standard SOM
Geographical error	1.1800	1.6713
Quantization error	7.1130	0.9030

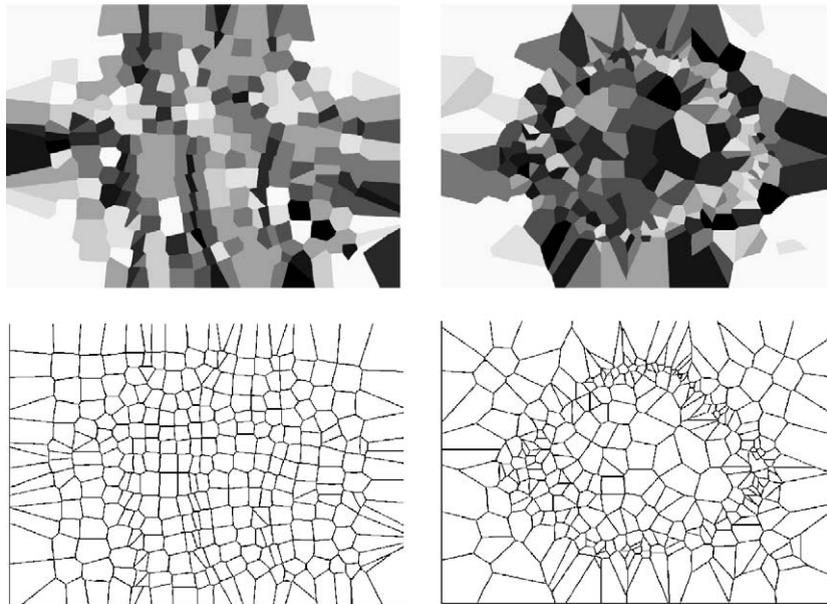


Fig. 7. Maps with average quantization error per unit (top), and geographical coverage of those units (bottom), using Geo-SOM with $k = 2$ (left) and standard SOM (right).

corner of the map has basically the same configuration as the other corners even though the data in that corner are significantly different. We may thus conclude that while the standard SOM may be a good clustering tool, it naturally fails to single out the geographical information contained in the data.

5. Practical application

For practical application, data from the Portuguese Institute of Statistics are used. These data refer to Lisbon's metropolitan area, and is at the enumeration district (ED) level, including 65 socio-demographic variables. These variables describe ED based on six main topics: information about buildings, families, households, age structure, education levels, and economic activities. Additionally, we introduced two explicitly geographic variables, representing the (x,y) coordinates of the geometric centroids of the EDs. The Geo-SOM was implemented in Matlab[®] compatible with Somtoolbox (Vesanto et al., 2000).

It is not our aim, at this point, to compare the quality of the results of each approach. Rather, the idea is to analyze the results especially in terms of their geographic context. The basic difference between the two approaches can be easily seen in Fig. 8. The Geo-SOM distributes the units according to two criteria: the geographic positioning of the input patterns (the ED's centroids), and the minimization of the quantization error of the units. This yields a distribution of the units that roughly follows the density of the input patterns but also takes into account their differences in terms of socio-economic variables. For example, if two areas have the same input pattern density, but in area A the similarities between the input patterns is higher than in area B, then area B will be granted a higher number of units. On the other hand, the standard SOM places the units solely based on the minimization of the quantization error. Because of this, the centre of the geographic map is very densely populated with units and very few are displaced to represent the characteristics of the periphery.

The possibility of using the Geo-SOM in the definition of homogeneous zones or in the identification of discontinuities in spatial data is particularly appealing. Bearing in mind that each unit has a geographic positioning and also an associated quantization error, a Voronoi partition based on the geographical distribution of the units can be made. This partition along with the quantization error allows us to identify zones where the change in characterization of the EDs happens. Fig. 9 shows such an example. The dark shaded polygons represent boundary areas. In fact, the analyses of the figure is in accordance with the reality of the city in the



Fig. 8. Geographic placement of SOM units for Geo-SOM (top) and standard SOM (bottom), units are represented by black points and EDs by light shaded squares.

sense that most of the areas represented as borders correspond to “de facto” borders. For instance, some of these areas represent large infrastructures such as the Lisbon airport where the number of input patterns is very scarce being surrounded by very different socio-economic zones.

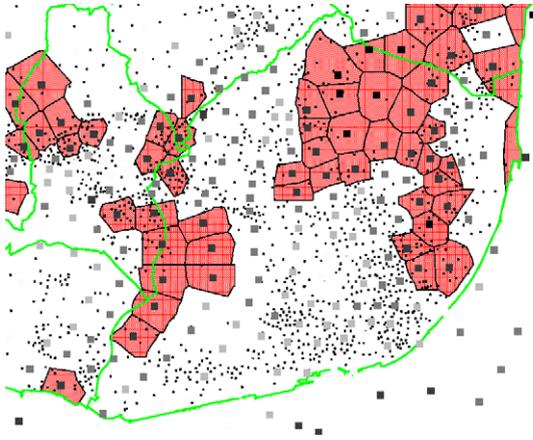


Fig. 9. Closeup of study region, showing areas with high quantization errors (in dark shades), geographical placement of SOM units (squares) and input data (circles).

6. Conclusions

In this paper we present a number of SOM variants that are particularly well suited to deal with geo-referenced data. The fundamental idea is to introduce spatial paradigms, such as spatial autocorrelation, into the workings of the standard SOM algorithm. We present the Geo-SOM, which enables the treatment of the spatial dimension of the data separately from other attribute data, when performing data reduction tasks. The Geo-SOM yields a coherent geographic distribution of the SOM units, according to the geographic density of the input patterns but also according to the similarity between neighbours. The potential of this new approach in the definition of homogeneous zones and the identification of borders is shown in an artificial data set and also in a real world application. We also wrote the Matlab software to implement these variations, which is available at <http://www.isegi.unl.pt/docentes/vlobo/projectos/programas/programas.html>. One of the major challenges in terms of future work in this area is to derive the relations established between geographic density and attribute space density by the Geo-SOM. Additionally, it is important to include other tools made available by the SOM, such as U-matrices, in the analysis of the results provided by this new approach.

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