Distance between Kohonen classes:

Visualisation of data set structure with Self Organising Map

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Running title: Chart of SOM classes distance

Preferred section: Technology and Applications

Abstract

Self Organising Map (SOM) is an often-used clustering method that mirrors the topology between classes with a map. Many tools superimpose on this map endogenous or exogenous information in order to integrate this topology in the data analysis. A new tool, that we present here, displays the results of the computation of the distances between all centroids, which simplifies the distance-matrix contents by managing the redundancy. Therefore, this tool allows an interpretation in the input space by visualising the intrinsic structure of the data. The SOM becomes then an efficient non-linear multidimensional data analysis method including graphical representations. As an application, the Kohonen map is used to chart any classification in the input space. This method is particularly well adapted when the intrinsic structure of the data is not linear at all, and can eventually supply classical linear techniques. Furthermore, SOM can be perceived as a technique of data set adjustment with a surface including its own graphical representation.

Keywords: Classification, Data set representation, Kohonen maps, Multivariate data analysis, Neural networks, SOM.

1. Introduction

Representation of information given by clustering methods is of little satisfaction. Some tools able to localise classes into the input space are expected in order to provide a good visual support to the analysis of classification results. Actually, clusters are often visualised with the planes produced by factor analysis (Wong, 1982; Lebart, Morineau & Piron, 1995). These representations are sometimes unsatisfying, for example when the intrinsic structure of the data is not at all linear or when the compression phenomenon generated by projections on factorial planes is very important. In the family of clustering methods, the Kohonen algorithm has the originality to organise classes considering the neighbourhood structure between them (Kohonen, 1993; Kohonen, 1995; Cottrell, Fort & Pagès, 1998). Many transcriptions in graphical displays have been conceived to optimise the visual exploitation of this neighbourhood structure (Cottrell & al., 1999; Rousset, 1999). Each one helps the interpretation in a particular context, they are twinned to the Kohonen algorithm and called *Kohonen maps*. For example, one used in the following helps the interpretation of the classification from an exogenous or endogenous qualitative variable. Unfortunately, no one allows for a visualisation of the data set structure in the input space. This is very regrettable when the Kohonen map makes such a folder that two classes close to each other in the input space seem to be far on the map. A tool that visualises distances between all classes (not only neighbouring classes) can detect some eventual folders. More generally, it gives a representation of the classification structure in the input space. Such a tool is proposed in the following. Two populations close in the input space but separated in different clusters are called *locally* distant. As on the one hand the Kohonen algorithm has the property to reveal effects of *local distances,* and, on the other hand the new tool is able to control large distances, this clustering method has now a large field of exploitation. When the previous Kohonen map charts the neighbourhood organisation between classes, this tool localises centroids in the input space, and then visualises the data set structure.

In the context of multidimensional analysis, the graphical display of all distances between classes transforms the Kohonen algorithm from a clustering technique summarising information into a data analysis and data set representing method (Blayo & Demartines, 1991; Cottrell & Ibbou, 1995; Wong, 1982). Its approach can be compared with factor analysis. In particular it can be used to study the result of any classification *c* (not only the Kohonen one). To avoid any confusion, in this paper the prefix *k* refers to the Kohonen algorithm and *c* or nothing refer to other classifications. As the distance chosen for the k-algorithm and for the c-classification are in coherence (Euclidean one for both, χ^2 for both, etc.), it is probable that any difference between individuals able to generate a c-class would also create a k-class. In that situation, the Kohonen map is probably more adapted to visualise some local distance influences than projections on planes that are more sensitive to large distances. This noticed property would reduce the very well known risk of compression induced by the association between the clustering method and a factor data analysis. The new technique is also presented as the approximation of the data set by a non-linear surface. One can use for example a Multilayer Perceptron to do it but in that case it is not very easy to interpret the model. At the contrary, the tool that charts the surface structure simplifies the interpretation and makes this method an easy one to use.

In the following the Kohonen map is used first as a method of classification which takes into account both proximity and remoteness. In a second time it is applied as a method of data analysis to represent the data set itself or one of its summaries such as the example of any other classification result. To illustrate the possibilities of this technique, we use the example of a data set concerning human healthy skin quality and resulting from a study performed by the C.E.R.I.E.S. The purpose of this study is to search for a typology of the human healthy skin out of several pertinent visual or tactile criteria. The data set consists in 17 criteria, assessed using ordinal scales, collected on a sample of 212 volunteer women. Some analyses have already been done on these data, each one corresponding to a different approach translated by adapted distance or referring method (Chavent, et al., 1999; Guinot, et al., 1997). As the assessment of the intensity of a skin feature is subjective, we decided to dichotomise each variable and to estimate the intensity from the frequency of the skin feature in each class. The underlying justification is the following: a cluster that contains a mixed population is considered well represented by an individual whose skin feature intensity corresponds to the percentage of this feature in this cluster, in a scale from 0 to 1. Therefore, the Euclidian metric was used to compute distances. First, the Kohonen algorithm with Euclidean distance is applied to classify individuals, then is used to represent in the input space the result of a hierarchical classification using the Ward distance.

2. Representation of individuals with the couple classification-factorial analysis

A classical method to visualise classification results consists in using factor analysis. All individuals are projected on the principal planes, their projections are pointed with a mark corresponding to their own class. The properties of this very common method are strongly linked to projections ones. In particular, it describes the clusters from a vectorial space smaller than the one that builds them. This implies to consider the problem of the projection representativity. For example, it is common that the projections of two classes populations are mixed in such a way that one cannot attribute a connected area of the plane to each class. In fact, this kind of representation is more pertinent to show effects of large distances between individuals than small distances. It is as well effective to reveal one criterion influence as it contributes to any class build but it is less sensitive when this influence is restricted to discriminate specifically two close classes. To generalise these remarks, we can say that this method is more adapted to visualise effects of *global* distances than of *local* ones.

To illustrate these phenomena, individuals belonging to the data set sample of the skin quality have been classified with a hierarchical clustering method using the Ward distance and projected on the first principal plane as in figure 1.a. The first component globally corresponded to features associated with vascular system of the skin, which we will refer to as "vascular profile" of the skin, and the second component corresponded to features associated with "oiliness" of the skin. Following clustering analysis, six clusters were identified from these principal components. We notice that classes 2 # and 6 % are separated from the others by the first principal axis towards negative values but we can notice that their projections are mixed (figure 1.b). The second axis divides classes 1) and 5 +. Class 3 ' is partially mixed with classes 1) and 2 #. One needs to be reminded that if classes 1) and 6 % are far from the rest on the plane this does not necessarily mean that they keep this property in the complete space.

[add fig. 1. a and fig.1. b]

3. The Kohonen classification and its associated map

In this chapter, the Kohonen algorithm is considered only as a clustering method adapted to any distance and is particularly interesting when local distances have to be taken into account. In the following, a class issued from a Kohonen classification is called *k-class* in order to exclude any confusion with a class issued from another technique. The Kohonen network presented here is a two-dimensional grid with n by n units, but the method allows the choice of any topological organisation of the network. We name U=n×n the number of units. After the learning, the weight vectors G_u, called code vectors, represent in the input space their corresponding unit u. The delicate problem of the learning is not addressed here, it is supposed to be successfully realised. Each individual is associated to the code vector, which is the closest in the input space. In this way, two individuals associated to the same code vector G_u are assigned to the same class k_u. U k-classes k_u are defined in such a way. They are represented by their corresponding code vector G_u in the input space and unit u on the network. This classification has the particularity to organise units on a chart called Kohonen map such as units neighbouring on the map correspond to code vectors that are close in the input space. Consequently, two individuals that belong to classes referring to neighbouring units are close in the input space. On the contrary, to be far on the chart does not mean anything concerning the proximity. In the following, the neighbourhood notion refers to the map localisation. The boxes organisation of figure 2 is a traditional representation of the Kohonen map in the case of a grid. The unit u_0 neighbours for the rays 0, 9 and 25 are respectively the unit u_0 itself, any unit of the square of 9 units centred on u_0 and any unit of the square of 25 units centred on u_0. As an example: at ray 1, unit 11 neighbours are units 3, 4, 5, 10, 11, 12, 17, 18, 19.

The Kohonen map allows a representation of some characteristics of a k-class and the generalisation to its neighbours. For example, the effect of an endogenous or exogenous qualitative variable Q can be visualised by including into each unit a pie reflecting the proportion of one modality occurrence in the class population, as shown in figure 2. The pie slice angle is $2 \times \pi \frac{n_{ik}}{n_{.k}}$, where n_{ik} is the number of individuals classified in the k-class k for which Q takes the i modality and $n_{.k}$ is the number of individuals affected to the class k. Figure 2 represents one endogenous criterion effect, "the skin is yellow or not". The Q variable is then the criterion corresponding variable. Two areas of neighbouring units are emerging, one is composed of units 1, 2, 8 and the other one of units 28, 34, 35, 41, 42, 48, 49. Moreover another area grouping mixed population is located in the 7, 14, 21 units area. Each skin feature can be plotted similarly.

[add fig. 2.]

The main problem of such a representation is that units are localised on the map at equal distance from their neighbours while their respective code vectors are not at equal distances in the input space. In this way, the intrinsic data set structure in the input space is omitted. In the skin quality sample, this expresses the visual impossibility to conclude if the "yellow skin" feature is present in two separated areas of the data set input space or only in one. The problem of the graphical display of the data set in the input space is the aim of the following section where the proposed solutions are expected to allow the choice of one area or two.

4. Representation of distances between all classes and visualisation of the intrinsic data set structure in the input space

In order to give an idea of the data set structure in the input space, one first modest idea has already been proposed in (Cottrell & Rousset, 1997) to visualise the importance of the proximity between k-classes by grouping code vectors with a new classification on these U vectors, for example the hierarchical clustering method using the Ward distance. A colour is associated to each new class called in the following *macro-class.* It is used for example to colour the background in each unit cell as shown in figure 3. In practice, this technique groups more often code vectors located on connected areas of the map which confirms the neighbouring topology. This method applied to the quality skin sample leads to the figure 3 where 6 macro-classes determine 6 connected areas of the map. The upper-left corner macro-class (cyan coloured) groups a number of k-classes (4) twice smaller than the down-left corner one (magenta coloured)(8). Moreover, code vectors can belong to two different macro-classes and be close in the input space at the same time. This remark implies that this technique does not allow the visualisation of proximity in the input space between the corner upper-left and bottom-right. So, the macro-classes use increases our knowledge of the map structure in the data set input space, but it is necessary to visualise distances between code vectors to be more precise in the description.

[add fig. 3.]

A first way to represent the distance between code vectors of neighbouring classes has already been proposed in (Cottrell & de Bodt, 1996). The concept consists in separating two neighbouring units borders with a space which width is in proportion with the distance between their corresponding code vectors, as in figure 4. This method allows a distinction between a population large enough to generate two macro-classes and two different populations' separation. But the information on distance is restricted to neighbouring classes, in particular the distance between two macro-classes centroids is not discerned. Moreover it is usual that largest distances separate some borders of macro classes but also some k-classes of the same macro-class. This technique applied to the skin quality sample leads to figure 4. It shows that the right border of the map (units 6, 7, 13, 14, 20, 21, 27, 28, 34, 35, 41, 42, 48, 49) is separated from the large area of the rest. But it is very difficult to see the structure of this large area as the aspect of uniformity is probably wrong. To illustrate a previous remark, one can notice that the distance between neighbouring classes 35 and 41 is one of the largest while they belong to the same macro-class. Moreover it is still impossible to conclude in favour of proximity or remoteness between individuals affected in both map opposite corners upper-left and bottom-right. In conclusion, this method is a simple way to give a first aspect of distances between classes but must be completed with a tool that represents any distance between two centroids in order to have a complete information on the input space structure.

[add fig. 4.]

Now the necessity is fit to represent distances between any classes, which constitutes U^2 values. U^2 is usually a very large number and this values representation has to use the neighbourhood organisation in order to group the redundant information. This condition is necessary to obtain a result that can be exploited. The natural way is to describe these distances with a new Kohonen map divided in *U* boxes of *U* divisions. The principal consists in assigning on the map a colour to each couple of k-classes *(u, u')* in such a way that the colour of the division *u'* of the *u*th box indicates the size of the distance *d(u, u')*. This visualisation is a pertinent tool to understand the data set structure. Figure 5 is the map of distances applied to the skin quality sample. Four colours are used, the darker the colour is as the corresponding distance is large. The first grid (upper-left) which represents distance between unit 1 and any else shows that the light units are on the upper-left corner area (its own macro class units 2, 8 and 9) or on the bottom-right one (42 and 49). Now we can conclude that the two opposite corners of the map *upper-left* and *bottom-right* are close on the input space and so any individuals whose skin has the criterion *yellow skin* are in the same space area. This last conclusion is impossible from any of the previous representations and show the power of this new tool. Moreover the properties revealed by the previous distance maps are still appearing. As example, we have previously notice that the right border is rather far from the rest, this property still appears in grid 27 and 28. But this time, the exception of the bottom-right corner which is far from the middle of the map but close to the corner upper-left is emerging. Moreover, this new map allows for an understanding of the large rest area structure (all map except the left border one). For example, with grids 10 and 31 we can see the opposition between the upper and bottom borders of the map. As both previous techniques are simple and give a good idea of the local structure, this new map is more complex to read but is more precise, gives a more complete visualisation of the data set structure, represents small and big distances and gives more security to the interpretation.

[add fig. 5.]

5. Any classification representation with a Kohonen map

In this section, the Kohonen algorithm result is perceived as a summary of the input data set in U points of this space and the different maps presented in sections 2 and 3 as a visualisation of the input data set structure. It is so natural in order to solve the initial goal to use these maps to represent any clustering method result and not the only Kohonen one. The distance choice is free which allows the use of one in coherency with the classification one. A qualitative variable Q is defined in order to affect to any individuals the index of its own class. This Q variable cartography done as in section 2 (figure 2) allows for the characterisation of any part of the input space from the clusters. A similar map can be build to localise any modality of the Q variable, and so any class, in the input space. Instead of the pie of figure 2, a bar chart represents the proportion between the contingency n_{ik} of the population *composed of individuals that belong to the class k and have the modality i* and the contingency $n_{i.}$ of the population *that has the modality i as common characteristic*. As the angle of the pie is $2 \times \pi \frac{n_{ik}}{n_{.k}}$, the size of the bar chart is $\frac{n_{ik}}{n_{i.}}$. Figure 7 is the result of this graphical technique applied to a classification in 6 classes. By cumulating contingency representation (figures 6 and 7) and distance maps information (figure 4 and 5), it is possible to have a large idea of the clusters repartition in the input space. On the figure 6 we can see that class 1 (pink circles) is a major component of a macro-class (pink rectangle), class 4 (grey circles) is almost totally included in an other macro-class (green rectangle), and class 5 (blue circles) is constitutive of a third macro-class (yellow rectangle). By contrast, class 3 (yellow circles) is spread into two macro-classes (blue and grey rectangles) and class 2 into four macro-classes. Similarly, the macro-class represented by the grey rectangles is composed of class 6 (green circles), a part of class 3 (yellow circles) and a part of class 2 (dark blue circles).

[add fig. 6.]

This method can be applied to the example of the healthy human skin quality to illustrate its possibilities to visualise for example the 6 grouping obtained at level 6 classes of a hierarchical classification using the Ward distance. Figures 7 and 5 show that individuals of classes 2 and 6 are in the right border and so far from the rest of the population. Class 6 is close from class 3 as it is located in the corner bottom-right. This class 3 is also present in the upper-left corner that is remained to be close from the bottom-right corner in the input space. Classes 1, 4 and 5 are constituting the main area of the map, the middle and the left side map except the upper-left corner. It looks as a large uniform population where classes 1 (bottom side) and 5 (upper side) are opposite and class 4 (middle) is the medium population. Moreover, class 3 is close from classes 1, 4, 5 and as well than from class 6 and appears also as a medium class for the data set.

[add fig. 7.]

6. Perspective

While code vectors are projected on a factorial plane and neighbouring unit ones are linked together, the representation obtained is the kind of figure 8. The colour indicates the macro-class. The links determine triangles that generate a surface. This surface adjusts the data set by joining any *U* code vector to its neighbours as in figure 9, except that in order to simplify the representation only 4 neighbours links are drawn. The data set representation with map previously presented in section 2, 3 and 4 can be considered as a graphical display of this surface and as well of any surface that adjusts the data set tying neighbouring code vectors. We have then on the one hand a way to summarise the data set structure with a surface and on the other hand some tools very well adapted to non-linear structure to visualise this surface.

[add fig. 8 and 9.]

7. Conclusion

We have presented a method to visualise the input data set structure with the Kohonen maps that is able to substitute linear graphical displays when these one are unsatisfying. While the Kohonen map reefers to the neighbourhood structure between the k-classes produced by this algorithm, a new tool that represents any distance between k-classes centroids allows for some of properties in the input space. This new technique can be applied to a larger domain than the interpretation of the k-classes. In particular in data analysis, it looks very well adapted to some applications such as the visualisation of any c-clustering result. In that context, the many charts associated to the Kohonen algorithm became also graphical displays of the data set or the c-clusters properties. For example, the one of figure 2 shows at the same time effects of any qualitative variable on the k-classification and on any clustering result. As a perspective, it can probably be used to visualise some adjustment of the data set with non-linear surfaces.

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Table 1: Schematic description of the classes.

Classification	Schematic description
Class 1)	Non-oily, pinkish skin colour, regular skin texture, redden upon touching
Class 2 #	Whitish skin colour, regular skin texture, redden only when pinched
Class 3 '	Yellowish skin colour, redden upon touching
Class 4 !	Pinkish skin colour, scaling, rough touch, irregular skin texture, redden upon touching
Class 5 +	Oily skin, pinkish skin colour, irregular skin texture, redden upon touching
Class 6 %	Non-oily, yellowish skin colour, irregular skin texture, do not redden even when pinched

Fig. 1. Combination between a principal component analysis and a hierarchical classification with the Ward distance.

a. Individuals are pointed by their own class mark (class 1) ; class 2 #; class 3 '; class 4 !; class 5 +; class 6 %).

a. The plane is split according to the schematic description of the axes and the classes repartition.

Fig. 2. Kohonen classification characterisation with a qualitative endogenous or exogenous variable, numeration is going from upper-left to bottom-right. Frequency of individuals where the criterion "yellow skin" is present or not corresponding to blue sector and pink sector, respectively.

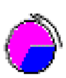

Example: 33% individuals of this class have a "yellow skin".

Fig. 3. Macro-classes representation is **added to the map of the criterion "yellow skin"**, (the 6-level groups of a hierarchical classification on the 49 code vectors realised with the Ward distance).

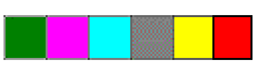

Macro-classes colour code.

Fig. 4. Representation of distance between neighbouring classes centroids.

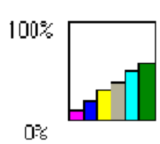
Fig. 5. Representation of any distance between centroids, grids and divisions has the same organisation than any previous Kohonen map.

 Colour code which represents distances.

Fig. 6. The k-classes obtained with the Kohonen algorithm are crossed with a hierarchical classification using Ward distance, they are both applied to the same data set. The contingency resulting is represented with the Kohonen map in order to integrate the associated topology. The contingency is measured in proportion of the k-classes individuals number and represented by the slice:

 Classes 1->6

Fig. 7. The k-classes obtained with the Kohonen algorithm are crossed with a hierarchical c-classification using Ward distance, they are both applied to the same data set. The contingency resulting is represented with the Kohonen map in order to integrate the associated topology. The contingency is measured in proportion of the c-classes individuals number and represented by the bar size.



Classes 1->6 Case 10% of class 1, 20% of class 2,..., 60% of class 6

Fig. 8. The surface generated by Kohonen classes centroids and links between them is projected on the first principal plane. To simplify the representation, only 4 neighbours links are drawn. The colour indicates the macro-class.

Fig. 9. The surface generated by Kohonen classes centroids and links between them is projected on a plane. To simplify representation, only 4 neighbours links are drawn: Map brim is overdrawn (the stippled design corresponds to the back part of the surface).

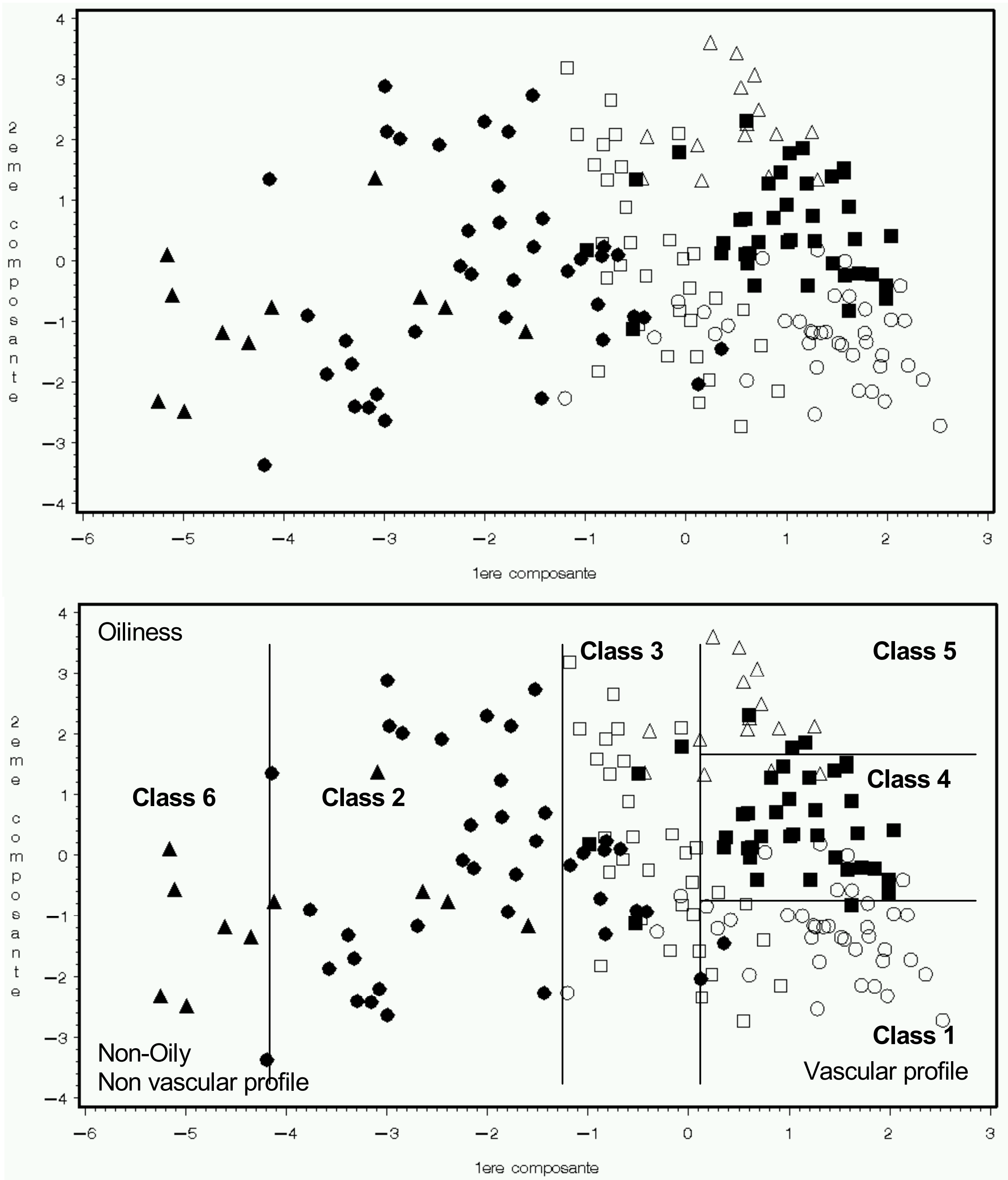
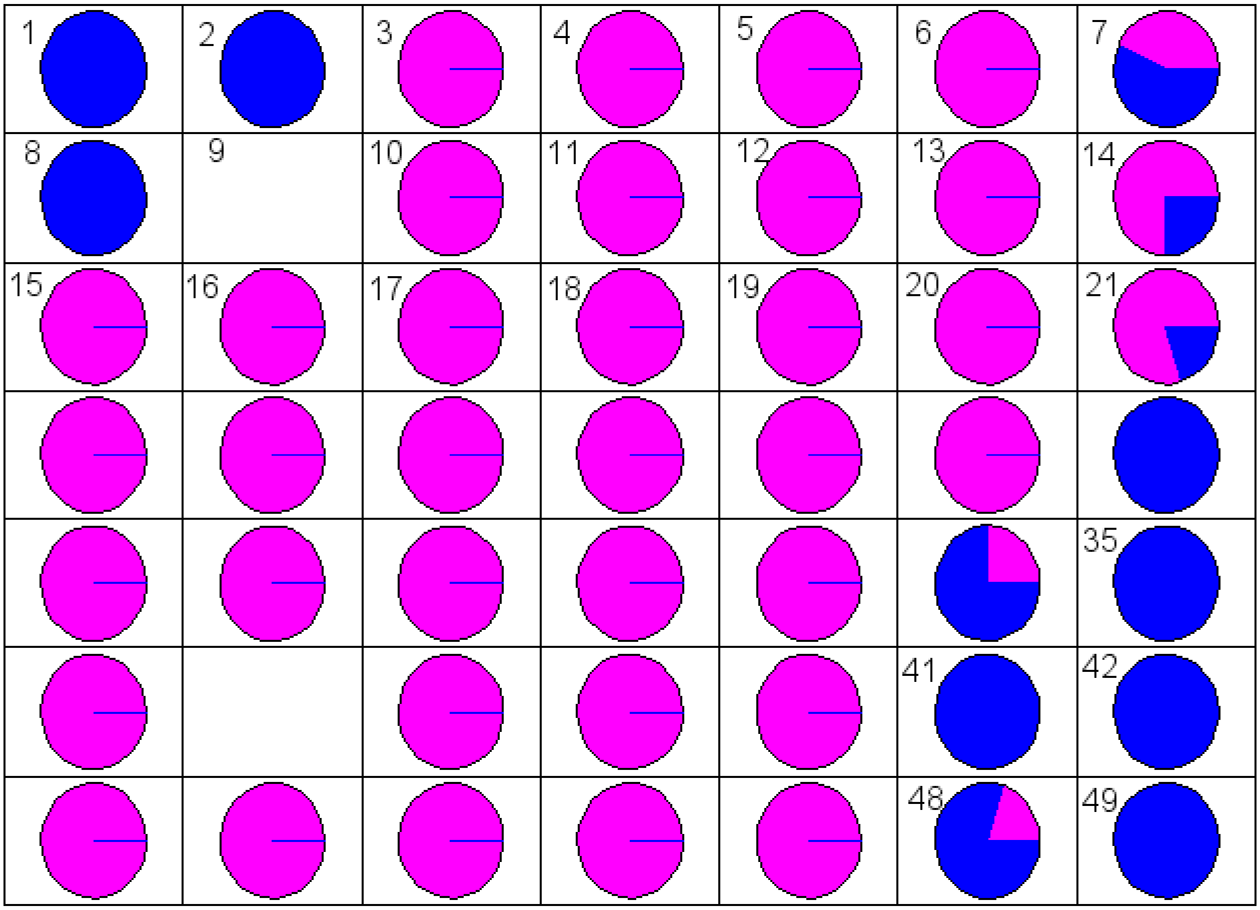


Fig. 1. Combination between a principal component analysis and a hierarchical classification with the Ward distance.

b. Individuals are pointed by their own class mark (class 1); class 2 #; class 3 '; class 4 !; class 5 +; class 6 %).

c. The plane is split according to the schematic description of the axes and the classes repartition on the plane.



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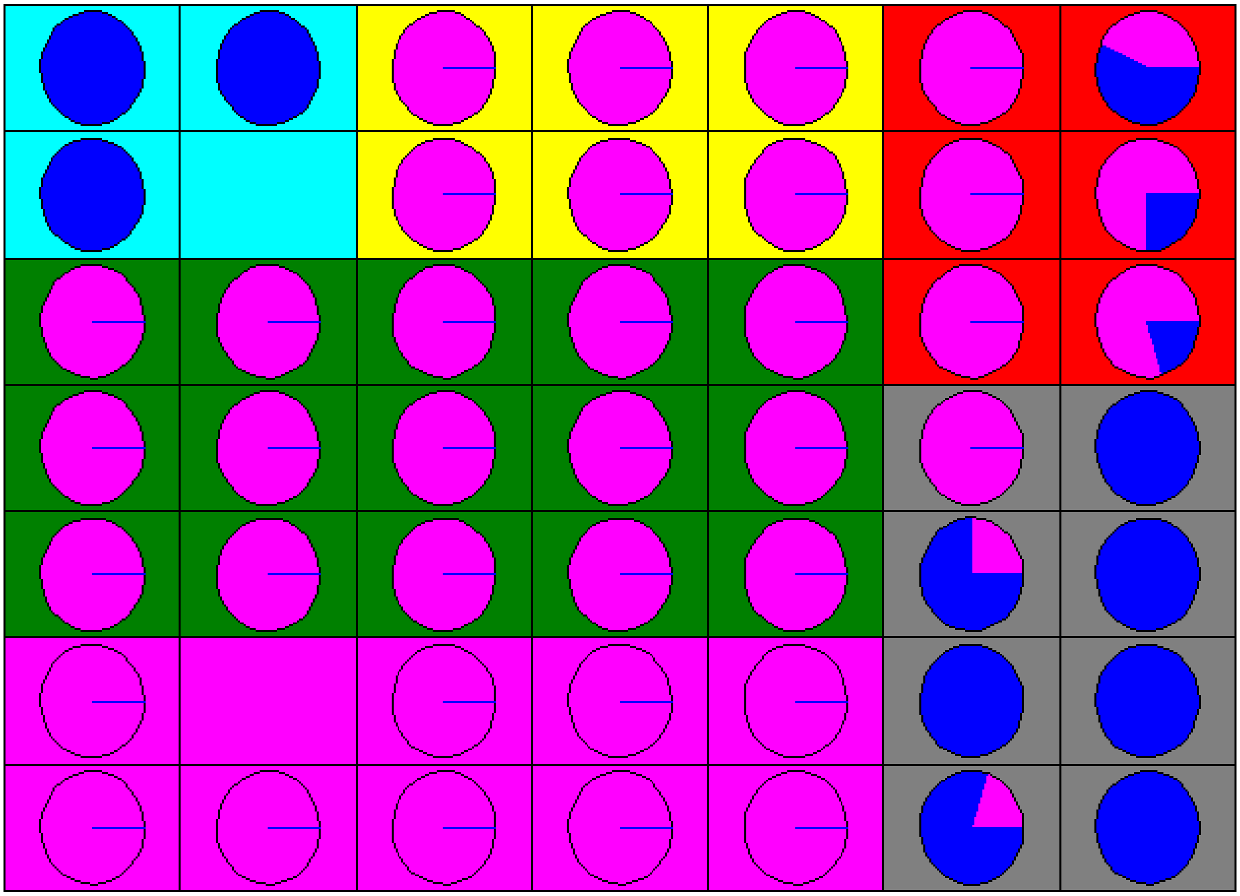
 Example: 33% individuals of this class have a "yellow skin".



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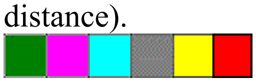
 Macro-classes colour code.

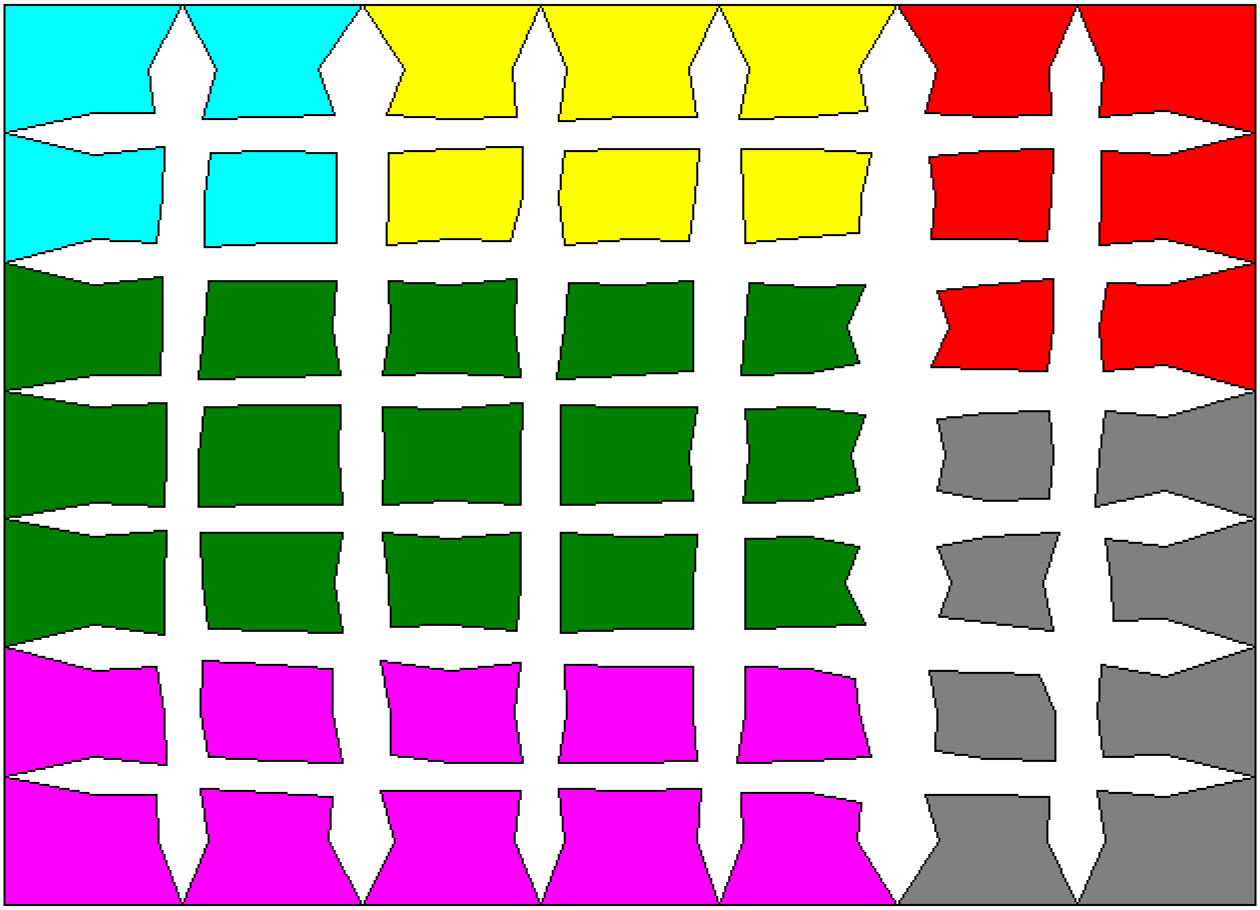


Fig. 4. Representation of distance between neighbouring classes centroids.

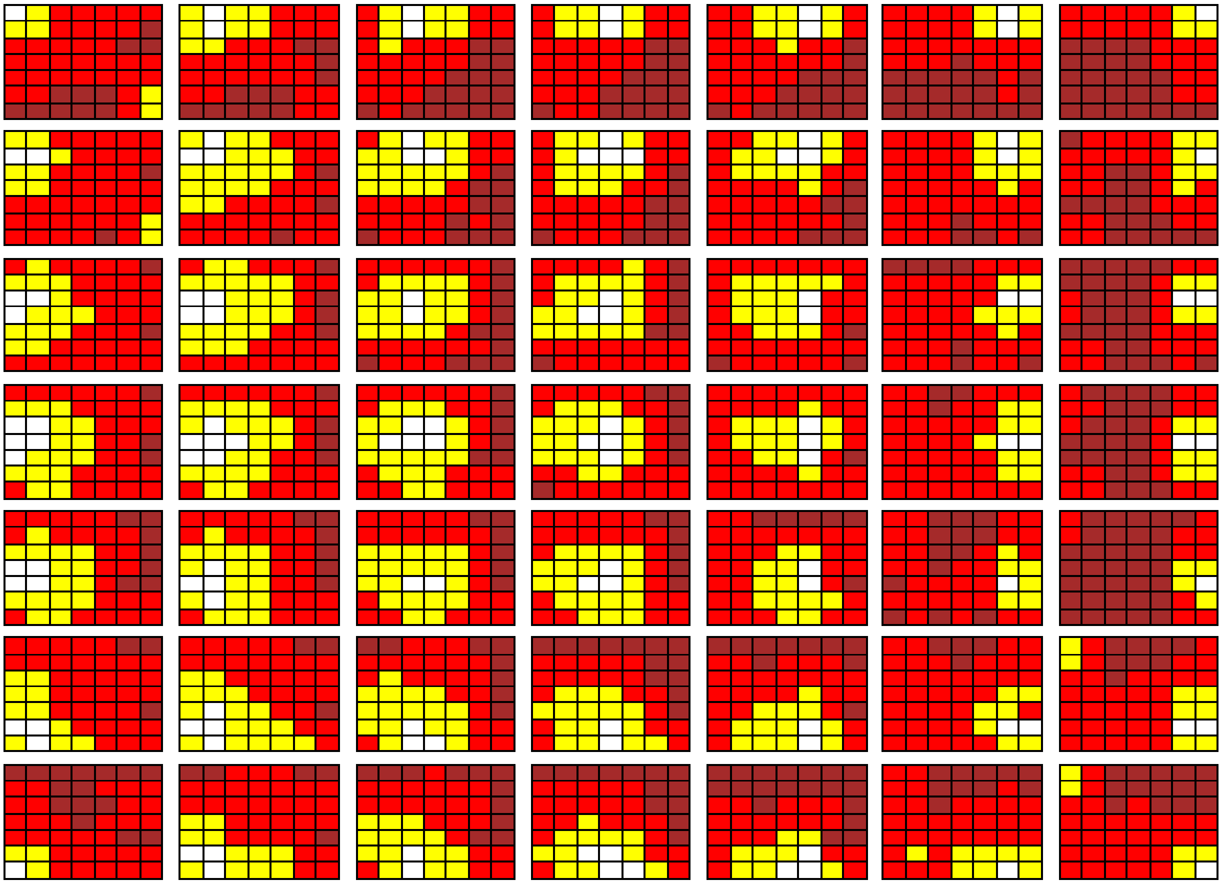
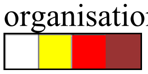


Fig. 5. Representation of any distance between centroids, grids and divisions has the same organisation than any previous Kohonen map.

 Colour code which represents distances.

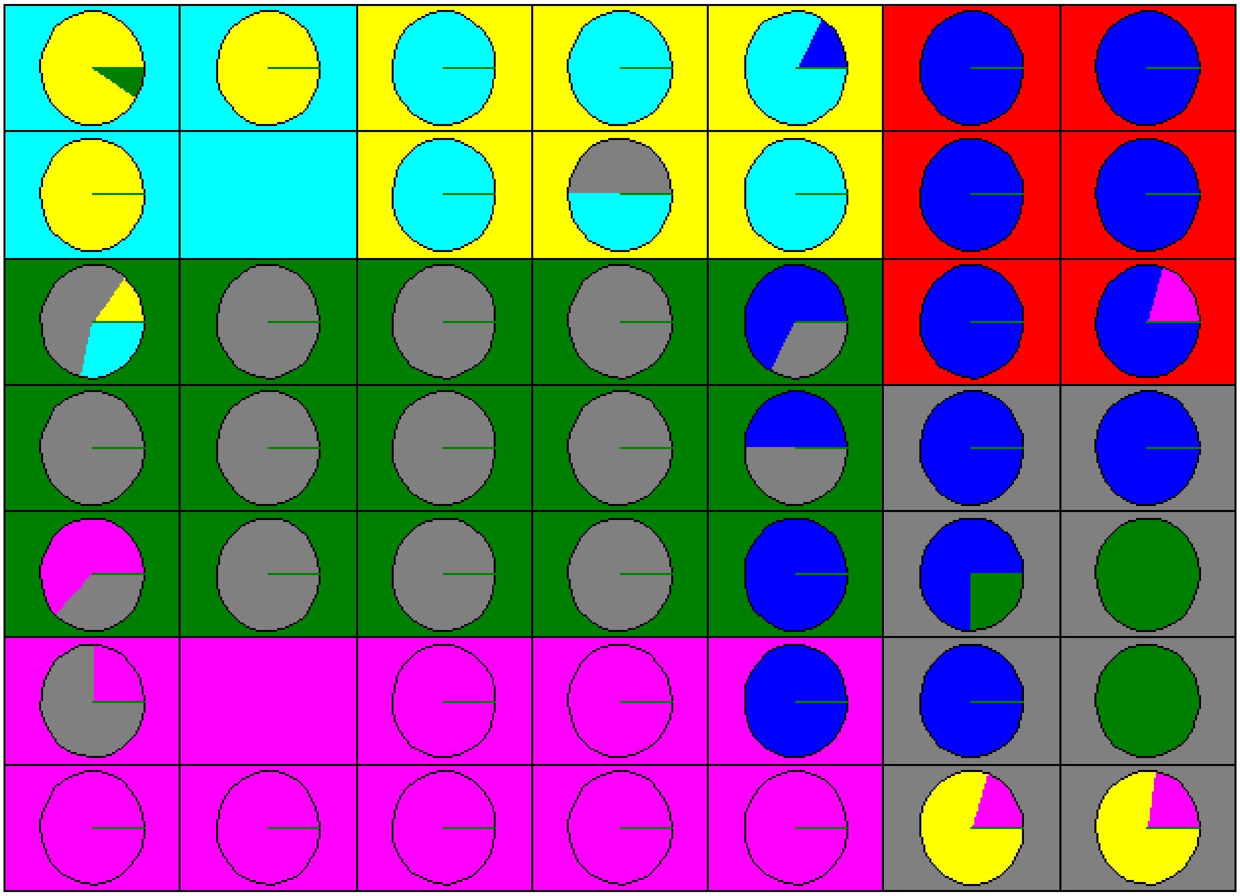


Fig. 6. The k-classes obtained with the Kohonen algorithm are crossed with a hierarchical classification using Ward distance, they are both applied to the same data set. The contingency resulting is represented with the Kohonen map in order to integrate the associated topology. The contingency is measured in proportion of the k-classes individuals number and represented by the slice:

 Classes 1->6

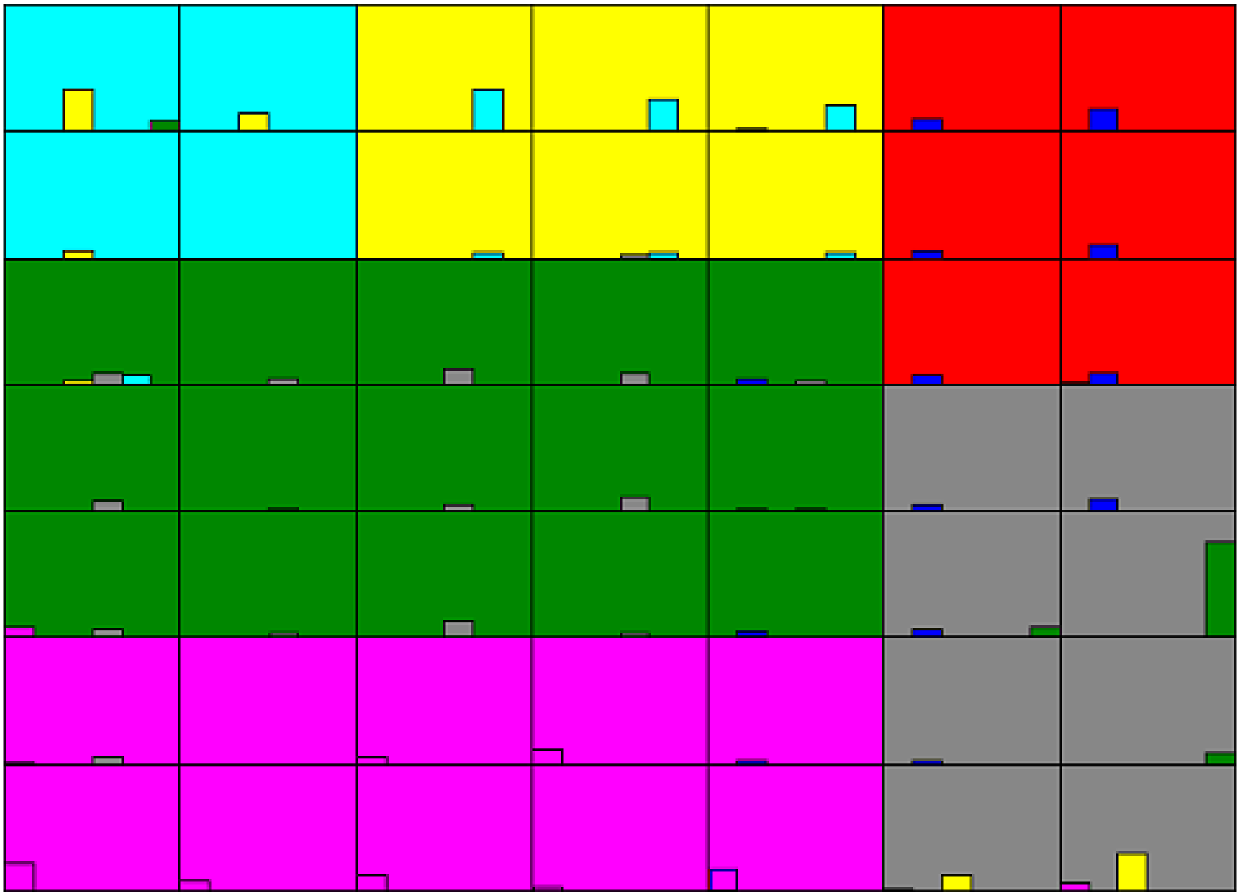
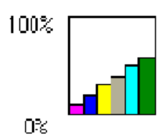


Fig. 7. The k-classes obtained with the Kohonen algorithm are crossed with a hierarchical c-classification using Ward distance, they are both applied to the same data set. The contingency resulting is represented with the Kohonen map in order to integrate the associated topology. The contingency is measured in proportion of the c-classes individuals number and represented by the bar size.



Classes 1->6 Case 10% of class 1, 20% of class 2,..., 60% of class 6

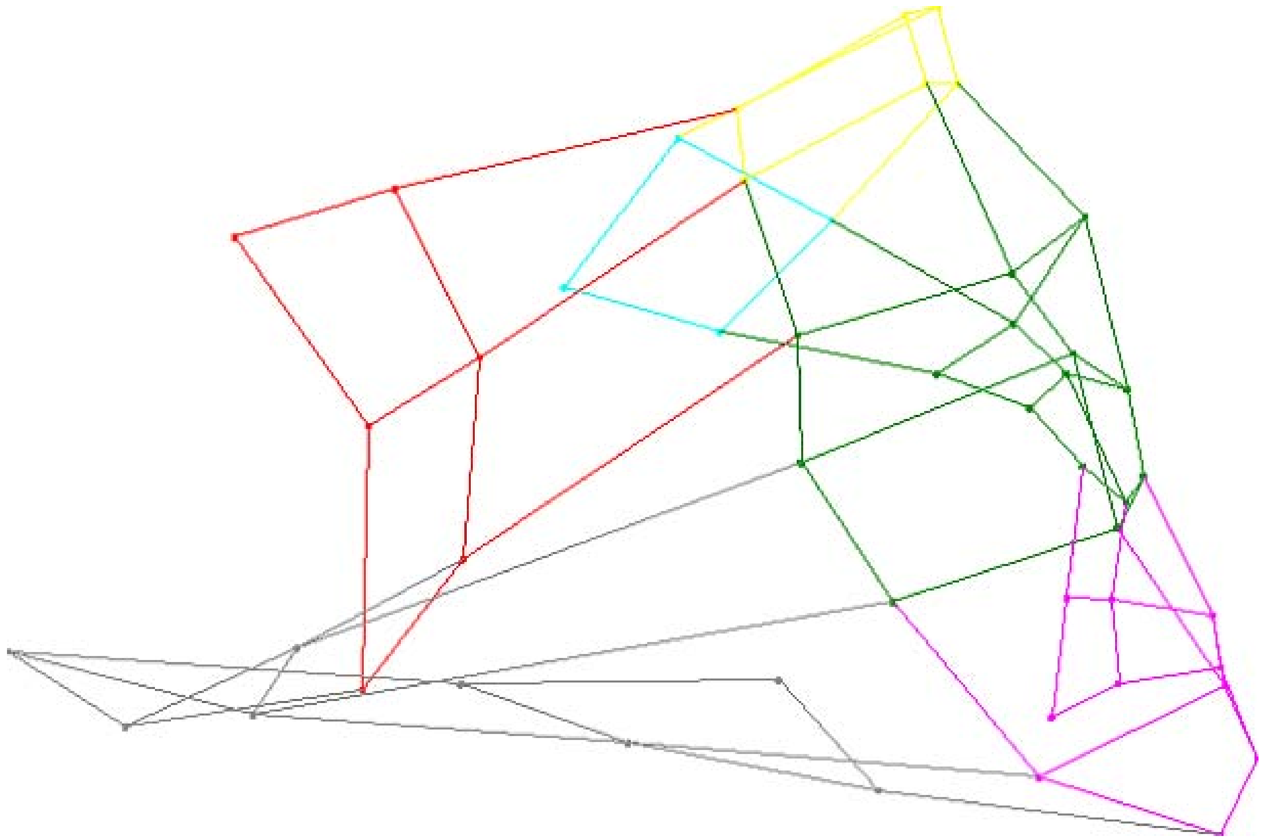


Fig. 8. The surface generated by Kohonen classes centroids and links between them is projected on the first principal plane. To simplify the representation, only 4 neighbours links are drawn. The colour indicates the macro-class.

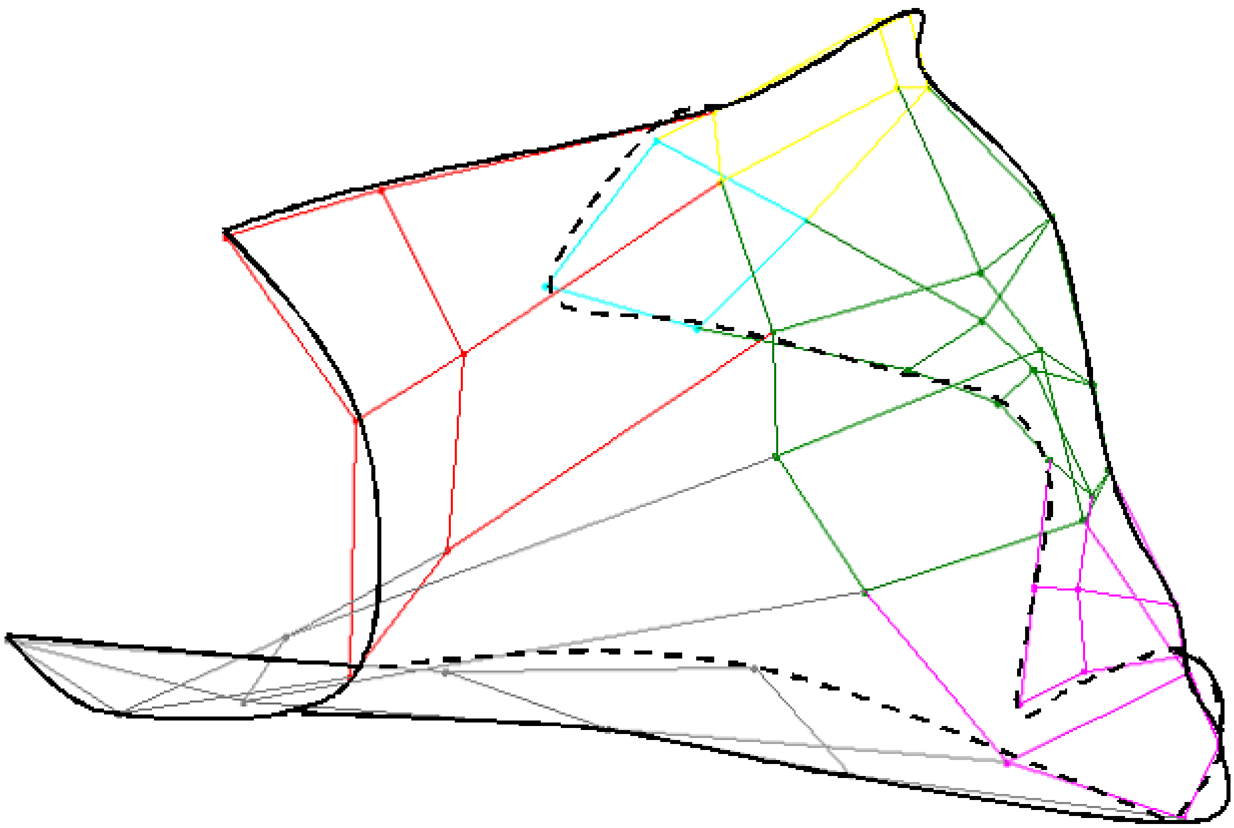


Fig. 9. The surface generated by Kohonen classes centroids and links between them is projected on a plane. To simplify representation, only 4 neighbours links are drawn: Map brim is overdrawn (the stippled design corresponds to the back part of the surface).