

SELF-ORGANIZING MAPS, THEORY AND APPLICATIONS

Marie Cottrell *, Madalina Olteanu *, Fabrice Rossi *, Nathalie Villa-Vialaneix **

*SAMM - Université de Paris I, France†

**INRA, MIA-T, INRA, Université de Toulouse, France.

ABSTRACT

The Self-Organizing Maps (SOM) is a very popular algorithm, introduced by Teuvo Kohonen in the early 80s. It acts as a non supervised clustering algorithm as well as a powerful visualization tool. It is widely used in many application domains, such as economy, industry, management, sociology, geography, text mining, etc. Many variants have been defined to adapt SOM to the processing of complex data, such as time series, categorical data, nominal data, dissimilarity or kernel data. However, so far, SOM has suffered from a lack of rigorous results on its convergence and stability. This article presents the state-of-art on the theoretical aspects of SOM, as well as several extensions to non numerical data and provides some typical examples of applications in different real-world fields.

KEYWORDS: SOM, Batch SOM, Stability of SOM, KORRESP, Relational and kernel SOM.

MSC: 68T10.

RESUMEN

El algoritmo de auto-organización (Self-Organizing Map, SOM), o Mapa de Kohonen, es un algoritmo muy popular, definido por Teuvo Kohonen al principio de los años 80. El actúa como un algoritmo de clasificación (*clustering*) no supervisado y al mismo tiempo como una herramienta potente de visualización. Es ampliamente usado para aplicaciones en muchos campos, tales como economía, industria, gestión, sociología, geografía, análisis de textos, etc. Muchas variantes han sido definidas para adaptar SOM al estudio de datos complejos, tales como series temporales, datos de categoría, datos nominales, datos de disimilaridades. Sin embargo, la convergencia y la estabilidad del algoritmo SOM no tienen pruebas rigurosas y completas hasta ahora. Este papel presenta el estado-del-arte de los aspectos teóricos de SOM, al mismo tiempo que algunas extensiones para datos no numéricos y ejemplos típicos de diferentes campos con datos reales.

PALABRAS CLAVE: Mapas auto-organizados, lotes de mapas auto-organizados, estabilidad de mapas auto-organizados, KORRESP, mapas auto-organizados kernels y relacionales

1. INTRODUCTION

This review is widely inspired by an invited paper [18] presented during the WSOM 2016 Conference, at Houston (USA) in January 2016, which addressed the Theoretical and Applied Aspects of the Self-Organizing Maps.

The self-organizing map (SOM) algorithm, defined by T. Kohonen in his first articles [40], [39] is a very famous non-supervised learning algorithm, used by many researchers in different application domains (see e.g. [37, 53] for surveys). It is used as a powerful clustering algorithm, which, in addition, considers a neighborhood structure among the clusters. In this way, close data belong to the same cluster (as in any other clustering algorithm) or to neighboring clusters. This property provides a

[†]marie.cottrell, madalina.olteanu, fabrice.rossi@univ-paris1.fr

good visualization of multidimensional data, since the clusters can be displayed according to their neighborhood structure. Furthermore, the SOM algorithm is easy to implement and as its complexity is linear with respect to the number of data, it is well-adapted to *Big Data* problems.

Its basic version is an *on-line* stochastic process, inspired by biological paradigms as it was explained in the first Kohonen's articles. It models the plasticity of the synaptic connections in the brain, where the neural connections either strengthen or disappear during "learning" phases, under the control of the practical experience and received inputs, without supervision.

For industrial applications, it can be more convenient to use a deterministic version of SOM, in order to get the same results at each run of the algorithm when the initial conditions and the data remain unchanged. To address this issue, T. Kohonen has introduced the batch SOM in [42, 44].

Over time, the researchers have defined many variants of SOM, some of them will be presented below. First the modified versions of SOM meant to achieve the goal of overcoming some theoretical difficulties of the original algorithm. But nowadays, SOM variants are being designed to deal with non numerical data (categorical data, abstract data, similarity or dissimilarity indices, for example).

The paper is structured as follows: Section 2 focuses on the definition of the original SOM algorithm designed for numerical data and on the main mathematical tools that are useful for its theoretical study. Section 3 is devoted to the simplest case, the one-dimensional setting, for which the theoretical results are the most complete. The multidimensional case is addressed in Section 4 together with some real-world examples. Sections 5 and 6 are dedicated to the definition of Batch SOM and of other interesting variants. In Section 7, we show how it is possible to extend the original SOM to non numerical data, and we distinguish between the extensions to categorical data and to dissimilarity or kernel data. The conclusion in section 8 provides some directions to go further.

2. SOM FOR NUMERICAL DATA

Originally in [40] and [39], the SOM algorithm was defined for data described by numerical vectors which belong to a subset \mathcal{X} of an Euclidean space (typically \mathbb{R}^p). For some results, we need to assume that the subset is bounded and convex. Two different settings have to be considered from the theoretical point of view:

- *the continuous setting*: the input space \mathcal{X} in \mathbb{R}^p is modeled by a probability distribution with a density function f ,
- *the discrete setting*: the input space \mathcal{X} comprises N data points x_1, \dots, x_N in \mathbb{R}^p . Here the discrete setting means a finite subset of the input space.

The data can be stored or made available *on-line*.

2.1. Neighborhood structure

Let us take K units on a regular lattice (string-like for one dimension, or grid-like for two dimensions). If $\mathcal{K} = \{1, \dots, K\}$ and t is the time, a neighborhood function $h(t)$ is defined on $\mathcal{K} \times \mathcal{K}$. If it is not time-dependent, it will be denoted by h . It has to satisfy the following properties:

- h is symmetric and $h_{kk} = 1$,
- h_{kl} depends only on the distance $\text{dist}(k, l)$ between units k and l on the lattice and decreases with increasing distance.

Several choices are possible, the most classical is the *step function* equal to 1 if the distance between k and l is less than a specific radius (this radius can decrease with time), and 0 otherwise.

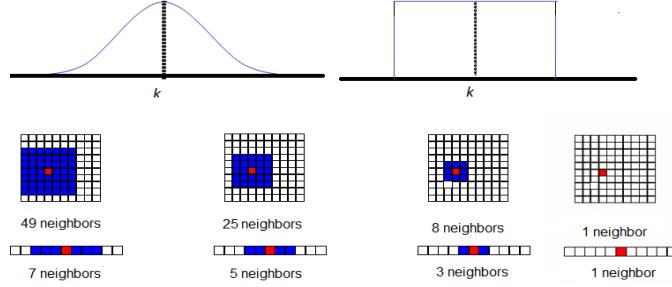


Figure 1: Neighborhood functions

Another very classical choice is a *Gaussian-shaped function*

$$h_{kl}(t) = \exp\left(-\frac{\text{dist}^2(k, l)}{2\sigma^2(t)}\right),$$

where $\sigma^2(t)$ can decrease over time to reduce the intensity and the scope of the neighborhood relations. For example, Figure 1 shows some classical neighborhood functions.

2.2. On-line SOM

A prototype $m_k \in \mathbb{R}^p$ is attached to each unit k , the initial values of the prototypes are chosen at random and denoted by $m(0) = (m_1(0), \dots, m_K(0))$. The SOM algorithm (in its *on-line stochastic version*) is defined as follows:

- At time t , a data point x is *randomly drawn* (according to the density function f (*continuous setting*) or in the finite set \mathcal{X} (*discrete setting*)),
- *The Best Matching Unit is defined by*

$$c^t(x) = \arg \min_{k \in \{1, \dots, K\}} \|x - m_k(t)\|^2, \quad (2.1)$$

- *All the prototypes are updated via*

$$m_k(t+1) = m_k(t) + \varepsilon(t) h_{kc^t(x)}(t)(x - m_k(t)), \quad (2.2)$$

where $\varepsilon(t)$ is a learning rate (positive, <1, constant or decreasing).

After learning, cluster C_k is defined as the set of inputs closer to m_k than to any other one. The result is a data space partition (Figure 2), called Voronoï tessellation, with a neighborhood structure between the clusters. The Kohonen map is the representation of the prototypes or of the cluster contents displayed according to the neighborhood structure.

The properties of the Kohonen maps are of two kinds:

- *the quantization property*, i.e. the prototypes represent the data space as accurately as possible, as do other quantization algorithms;
- *the self-organization property*, that means that the prototypes preserve the topology of the data: *close inputs* belong to the *same cluster* (as do any clustering algorithms) or to *neighboring clusters*.

To get a better quantization, the learning rate ε decreases with time as well as the scope of the neighborhood function h .

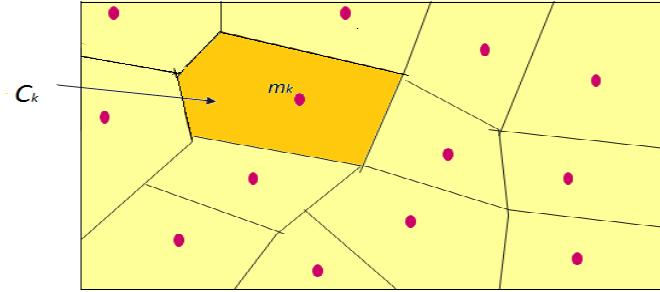


Figure 2: $c^t(x) = k \iff m_k(t)$ is the winning prototype of x

2.3. Theoretical concerns

The algorithm is, therefore, very easy to define and to use, and a lot of practical studies confirm that it works. But, in fact, the theoretical study of its convergence when t tends to $+\infty$ remains without complete proof and provides open problems ([8] and [25]). Note that this problem departs from the usual convergence problem addressed in Machine Learning Theory, where the question is to know if the solution obtained from a finite sample converges to the true solution that might be obtained from the true data distribution.

When t tends to $+\infty$, the \mathbb{R}^p -valued stochastic processes $(m_k(t))_{k=1,\dots,K}$ can present *oscillations*, *explosion* to infinity, *convergence in distribution* to an equilibrium process, *convergence in distribution or almost sure* to a finite set of points in \mathbb{R}^p , etc.

Some of the open questions are:

- Is the algorithm convergent in distribution or almost surely, when t tends to $+\infty$?
- What happens when ε is constant? when it decreases?
- If a limit state exists, is it stable?
- How to characterize the organization?

2.4. Mathematical tools

The convergence problem of SOM can be addressed with tools usually used to study the stochastic processes. One can emphasize on three main theories.

- *The Markov Chain theory* for constant ε and h , to study the convergence and the limit states.
 - If the algorithm converges in distribution, this limit is an *invariant measure* for the Markov Chain;
 - If there is strong organization, it has to be associated to an *absorbing class*.
- *The Ordinary Differential Equation method* (ODE)

If for each $k \in \mathcal{K}$, Equation (2.2) is written in a vector form:

$$m(t+1) = m(t) - \varepsilon(t)\Phi(x, m(t)), \quad (2.3)$$

where Φ is a stochastic term, then the ODE (Ordinary Differential Equation) which describes the *mean behavior* of the process is

$$\frac{dm}{dt} = -\phi(m), \quad (2.4)$$

where $\phi(m)$ is the expectation of $\Phi(., m)$.

Then the k^{th} -component of ϕ is

$$\phi_k(m) = \sum_{j=1}^K h_{kj} \int_{C_j} (x - m_k) f(x) dx \quad (2.5)$$

for the *continuous setting* or

$$\phi_k(m) = \frac{1}{N} \sum_{j=1}^K h_{kj} \sum_{x_i \in C_j} (x_i - m_k) = \frac{1}{N} \sum_{i=1}^N h_{kc(x_i)} (x_i - m_k) \quad (2.6)$$

for the *discrete setting*.

Therefore the possible limit states are solutions of the equation

$$\phi(m) = 0.$$

If the zeros of function ϕ are minimum values of a function (called Energy Function), one can apply the gradient descent methods to compute the solutions.

- The *Robbins-Monro algorithm* theory is used when the learning rate decreases under the conditions

$$\sum_t \varepsilon(t) = +\infty \text{ and } \sum_t \varepsilon(t)^2 < +\infty. \quad (2.7)$$

Despite the power of these mathematical tools, the original SOM algorithm is difficult to study for several reasons:

- for $p > 1$, it is not possible to define *any absorbing class* which could be an organized state;
- although $m(t)$ can be written down as a classical stochastic process, Erwinn et al., 1992, [22, 23], have shown that it does not correspond to any energy function, or in another words that the SOM algorithm is not a gradient descent algorithm in the continuous setting;
- finally, no demonstration takes into account the variation of the neighborhood function. All the existing results are valid for a fixed scope and intensity of the function h .

3. THE ONE-DIMENSIONAL CASE

This case is very simplified and far from the applications: the dimension $p = 1$, the data space $\mathcal{X} = [0, 1]$, the neighborhood structure is a string lattice, the data is distributed according to a uniform density and the parameter ε is constant. But it is the first case totally rigorously studied by Cottrell and Fort in 1987 [7].

They prove the following results:

Theorem 3.1. Simplest case

If ε is a constant $< 1/2$ and if the neighborhood of k is $\{k - 1, k, k + 1\}$,

- The number of badly ordered triplets is a decreasing functional;
- The set of ordered sequences (increasing or decreasing sequences, i.e. organized ones) is an absorbing class;
- The hitting time of the absorbing class is almost surely finite;

- The process $m(t)$ converges in distribution to a monotonous stationary distribution which depends on ε .

Figure 3. illustrates the first part of the theorem. The neighbors of j are $j - 1$ and $j + 1$. The values of the prototypes are on the y -axis, in $[0, 1]$. On the left, the first two triplets are not ordered. SOM will order them with a strictly positive probability. At right, the last two triplets are well ordered and SOM will never disorder them.

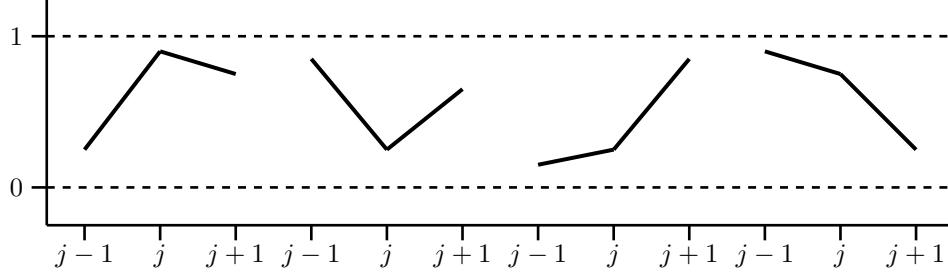


Figure 3: Four examples of triplets of prototypes, (m_{j-1}, m_j, m_{j+1})

Another result is available in the same frame, but when ε is decreasing, see [7].

Theorem 3.2. Decreasing ε

If $\varepsilon(t) \rightarrow 0$ and satisfies the Robbins-Monro conditions

$$\sum_t \varepsilon(t) = +\infty \text{ and } \sum_t \varepsilon(t)^2 < +\infty, \quad (3.1)$$

after ordering, the process $m(t)$ a.s. converges towards a constant monotonous solution of an explicit linear system.

Some results about organization and convergence have been obtained a little later by Bouton, Fort and Pagès, [6, 27], in a more general case.

Theorem 3.3. Organization

One assumes that the setting is continuous and that the neighborhood function is strictly decreasing from a certain distance between the units.

- The set of ordered sequences (increasing or decreasing sequences, i.e. organized ones) is an **absorbing class**;
- If ε is constant, the hitting time of the absorbing class is **almost surely finite**.

Theorem 3.4. Convergence

One assumes that the setting is continuous, the density is log-concave, the neighborhood function is time-independent and strictly decreasing from a certain distance between units.

- If the initial state is ordered, there exists a unique stable equilibrium point (denoted by x^*);
- If ε is constant and the initial disposition is ordered, there exists an invariant distribution which depends on ε and which concentrates on the Dirac measure on x^* when $\varepsilon \rightarrow 0$;
- If $\varepsilon(t)$ satisfies the Robbins-Monro conditions (3.1) and if the initial state is ordered, then $m(t)$ is almost surely convergent towards this unique equilibrium point x^* .

It is clear that even in the one-dimensional case, the results are not totally satisfactory. Although the hypotheses on the density are not very restrictive, some important distributions, such as the χ^2 or the power distribution, do not fulfill them. Furthermore, nothing is proved, neither if $\varepsilon(t)$ is a decreasing function to ensure ordering and convergence simultaneously, nor for a neighborhood function with a decreasing scope, whereas in practical implementations it is always the case.

4. THE MULTIDIMENSIONAL CASE

In the multidimensional case, most of the previous results do not hold. For example, no absorbing class has been found when the dimension is greater than 1. Figure 4. is an illustration of such case, in dimension 2 with 8 neighbors: even if the x - and y - coordinates are ordered, it is possible (with positive probability) to disorder the prototypes.

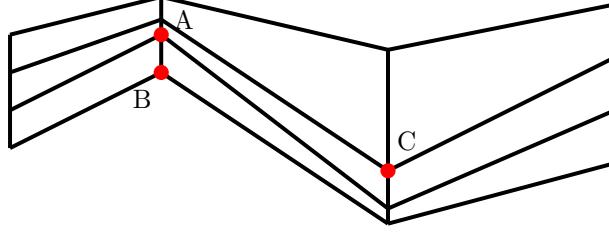


Figure 4: Disordering an ordered configuration. A is a neighbor of C, but B is not a neighbor of C. If C is very often the best matching unit, B is never updated, whereas A becomes closer and closer to C. Finally, the y - coordinate of A becomes smaller than that of B and the disposition is disordered.

However, some results are available, as shown below.

4.1. Continuous setting

Let p be the data dimension. Assume that h and ε are constant. Sadeghi (2001) [60] proves the following result:

Theorem 4.1. *If the probability density function f is positive on an interval, the algorithm weakly converges to a unique probability distribution which depends on ε .*

Assuming $p = 2$ and denoting by F^{++} the set of the prototypes with simultaneously increasing coordinates, these two apparently contradictory results hold.

Theorem 4.2. *For a constant ε and very general hypotheses on the density f ,*

- the hitting time of F^{++} is finite with a positive probability (Flanagan, 1996, [24]);
- but in the 8-neighbor setting, the exit time is also finite with positive probability (Fort & Pages, 1995, [26]).

However, in practical applications, the algorithm converges towards a stable equilibrium!

4.2. Discrete setting

For the continuous setting, we know that *SOM is not a gradient descent algorithm* (Erwinn, 1992, [22, 23]). But the discrete setting is quite different, since the stochastic process $m(t)$ derives from an energy function (if h is not time-dependent). This is a very important result, since in applications such as data mining or clustering, the data is always discrete.

For the discrete setting, Ritter et al., 1992, [57], prove the next theorem:

Theorem 4.3. *In the discrete setting, SOM is a gradient descent process associated to*

$$E(m) = \frac{1}{2N} \sum_{i=1}^N \sum_{k=1}^K h_{kc(x_i)} \|m_k - x_i\|^2, \quad (4.1)$$

called Extended Distortion or Energy Function.

Note that this energy function can also be written in a more explicit manner as

$$E(m) = \frac{1}{2N} \sum_{k=1}^K \sum_{j=1}^K h_{kj} \sum_{x_i \in C_j} \|m_k - x_i\|^2. \quad (4.2)$$

This result *does not ensure the convergence*, since the gradient of the energy function is not continuous on the boundaries of the clusters. But this energy has an intuitive meaning, because it combines two criteria : a clustering criterion and a correct organization criterion.

Note that in the 0-neighbor setting, SOM reduces to the Vector Quantization process (VQ), the energy reduces to the classical distortion (or within-classes sum of squares)

$$E(m) = \frac{1}{2N} \sum_{i=1}^N \|m_{c(x_i)} - x_i\|^2.$$

The gradient is continuous and in this case, the algorithm converges to one of the local minima.

4.3. Examples of practical applications

Figures 5 and 6 present some examples of Kohonen maps. The prototypes are displayed on the lattice and clustered into super-classes easier to describe, by using a Hierarchical Classification. The organization is confirmed since the super-classes group only neighboring prototypes.

In Ex. 1 (Figure 5) [9], there are 1783 districts in the French Rhône Valley, the dimension is 7, the variables are 7 census collected in 1936, 1954, 1962, 1968, 1975, 1982, 1990. The Kohonen map is a 8×8 grid. The data are grouped into 5 super-classes using a Hierarchical Clustering of the 8×8 prototypes. For Ex. 2 [49], in a week, at each quarter-hour, a binary code is filled by each worker: 1 if he works, 0 otherwise. Each observation is a $4 \times 24 \times 7 = 672$ -dimensional vector and there are 566 workers. The Kohonen map is a 10-units string, and the figure shows the 10 prototypes, grouped into 5 super-classes. In Ex. 3 [15], one sees the 10 colored super-classes, and below all the manuscript digits coded as 256-dimensional vectors are drawn in the Kohonen classes.

In Ex. 4 (Figure 6) [3] [12], 96 countries are described by 7 ratios (annual population growth, mortality rate, illiteracy rate, population proportion in high school, GDP per head, unemployment rate, inflation rate) in 1996. The prototypes are displayed on a 6×6 Kohonen map and grouped into 7 super-classes.

Ex. 5 [9] concerns the distribution of Canadian consumers based on 20 consumption categories. And Ex. 6 [10] displays the contents of each Kohonen class, on a 10×10 cylindrical map, after learning, where each observation is the daily electrical consumption in France measured each half an hour over 24 hours over 5 years.

5. DETERMINISTIC BATCH SOM

In some practical applications, it is preferable to use a deterministic version of SOM, in order to get reproducible results when the initial prototype values are fixed, [42, 44].

The idea is to compute the solutions directly, without any on-line learning and to use all the data at each iteration. It is known that the possible limit states of the SOM algorithm are solutions of the ODE equation $\phi(m) = 0$, so it is natural to solve it.

For the *continuous setting*, one gets

$$m_k^* = \frac{\sum_{j=1}^K h_{kj} \int_{C_j} x f(x) dx}{\sum_{j=1}^K h_{kj} \int_{C_j} f(x) dx}.$$

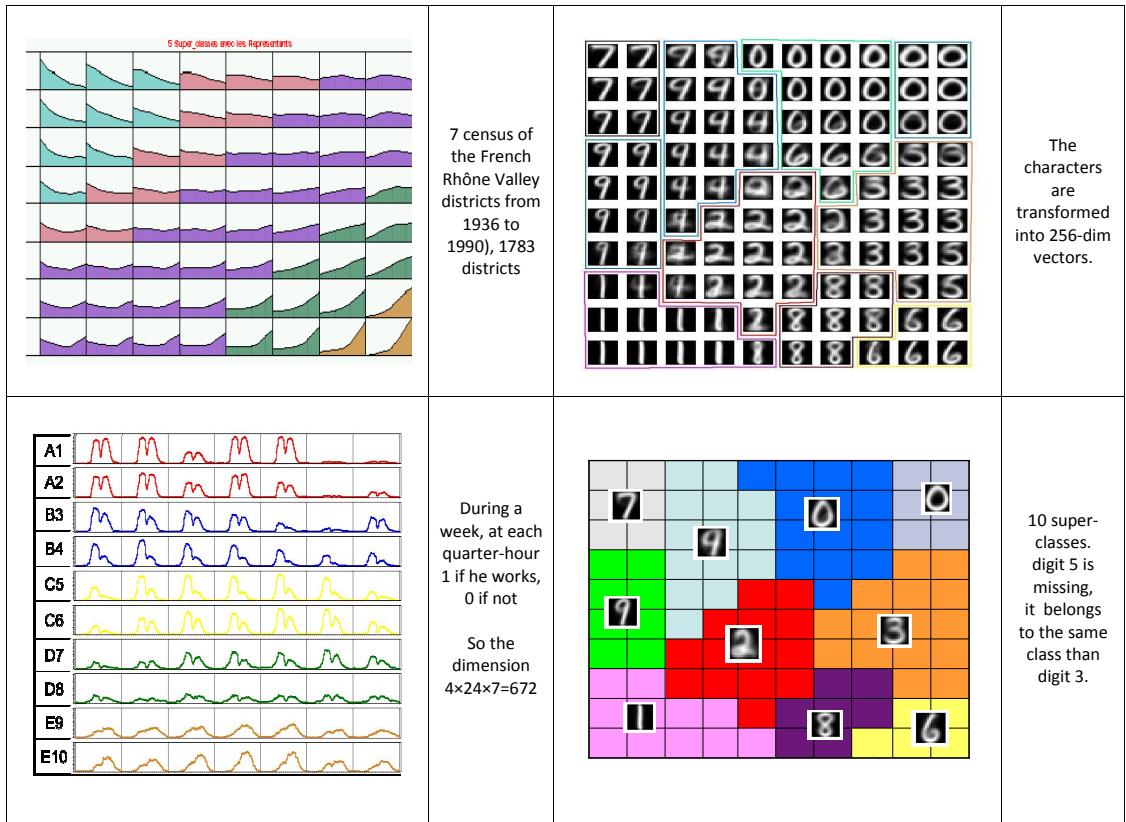


Figure 5: Ex. 1: clustering of districts (top left), Ex.2: workers schedules (bottom left), Ex. 3: manuscript characters (the super-classes at top right and the contents on bottom right).

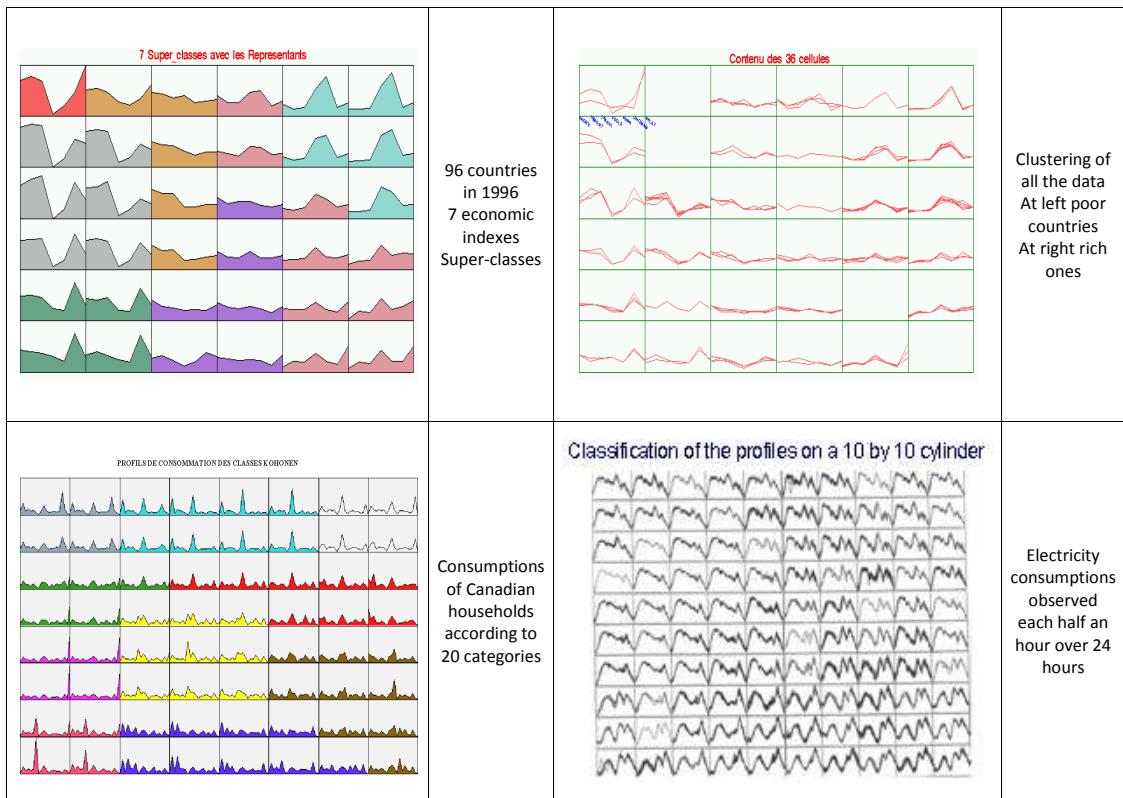


Figure 6: Ex. 4: countries (the prototypes on top left and the contents on top right), Ex. 5: domestic consumption (the prototypes on bottom left), Ex. 6: power consumption (the contents on bottom right).

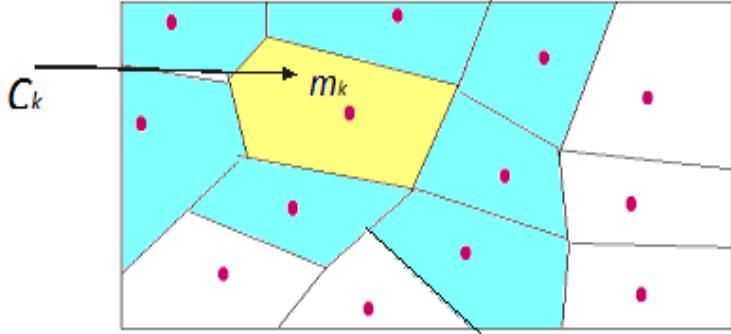


Figure 7: Batch SOM

and *in the discrete setting*, the analogous is

$$m_k^* = \frac{\sum_{j=1}^K h_{kj} \sum_{x_i \in C_j} x_i}{\sum_{j=1}^K h_{kj} |C_j|} = \frac{\sum_{i=1}^N h_{kc(x_i)} x_i}{\sum_{i=1}^N h_{kc(x_i)}}.$$

Therefore, the limit prototypes m_k^* are the weighted means of all the inputs which belong to the cluster C_k or to its neighboring clusters. The weights are given by the neighborhood function h . From this remark, Kohonen [42, 44], derives the definition of the Batch SOM, which directly computes the limit prototypes m_k^* , by

$$m_k(t+1) = \frac{\sum_{j=1}^K h_{kj}(t) \int_{C_j(m_k(t))} x f(x) dx}{\sum_{j=1}^K h_{kj}(t) \int_{C_j(m_k(t))} f(x) dx} \quad (5.1)$$

for the continuous setting, and

$$m_k(t+1) = \frac{\sum_{i=1}^N h_{kc^t(x_i)}(t) x_i}{\sum_{i=1}^N h_{kc^t(x_i)}(t)} \quad (5.2)$$

for the discrete case.

The initial values of the prototypes are chosen at random as usual. Figure 7 shows the limit prototypes as mean values of the union of its cluster and of the neighboring clusters.

For Batch SOM, the theory is a little more achieved, since it is proven by Fort et al., [28, 29], that it is a quasi-Newtonian algorithm associated to the Extended Distortion and that it converges to one of its local minima. Note that in the 0-neighbor setting, Batch SOM reduces to Forgy process (k -means, or what is also called Moving Centers), which converges towards a local minimum of the Distortion. Table 1 summarizes the relations between four clustering algorithms: the on-line SOM, the Batch SOM, the Vector Quantization (VQ) and the Forgy algorithm (or Moving Centers).

Some remarks highlight these relations:

- VQ and Forgy algorithms are 0-neighbor versions of on-line and Batch SOMs respectively;
- SOM and Batch SOM preserve the data topology: close data belong to the same cluster or to neighboring clusters;
- The Kohonen maps have good visualization properties whereas the 0-neighbor algorithms (Forgy and VQ) do not;

	Stochastic	Deterministic
0 neighbor	VQ, SCL	Forgy, Moving Centers
With neighbors	SOM	Batch SOM

Table 1: Comparison summary

- SOM depends very little on the initialization, whereas Batch SOM is very sensitive to it;
- Batch SOM is deterministic and often preferred for industrial applications.

6. VARIANTS OF SOM

Several variants have been defined to improve the SOM properties or to recast the SOM algorithm into a probabilistic framework.

6.1. Hard assignment in the Heskes'rule

One of the most important variants has been introduced by Heskes, 1999 [34], who has proposed a modification of the best-matching unit assignment, in order to get continuous gradient of the energy function.

Equation (1) is re-written

$$c^t(x) = \arg \min_{k \in \{1, \dots, K\}} \sum_{j=1}^K h_{kj}(t) \|x - m_k(t)\|^2. \quad (6.1)$$

With the Heskes rule, the energy function is continuous for both discrete and continuous settings, and its gradient is also continuous in the continuous setting. So this modified SOM is a gradient descent process of the Energy Function

$$E(m) = \frac{1}{2} \sum_{j=1}^K \sum_{k=1}^K h_{kj}(t) \int_{x \in C_j(m)} \|x - m_k(t)\|^2 f(x) dx. \quad (6.2)$$

in the continuous setting.

6.2. Soft Topographic Mapping - STM

The original SOM algorithm is based on a hard winner assignment. Generalizations based on soft assignments were derived in [31] and [34].

First we remark that the energy function in the discrete SOM can be written as:

$$E(m, c) = \frac{1}{2} \sum_{k=1}^K \sum_{i=1}^N c_{ik} \sum_{j=1}^K h_{kj}(t) \|m_j(t) - x_i\|^2,$$

where c_{ik} is equal to 1 iif x_i belongs to cluster k .

Then the crisp assignment is smoothed by considering $c_{ik} \geq 0$ such that $\sum_{k=1}^K c_{ik} = 1$, so that $c_{ik} = \mathbb{P}(x_i \in C_k)$.

Finally, a deterministic annealing scheme is used to avoid local minima: the energy function is transformed into a “free energy” cost function,

$$F(m, c, \beta) = E(m, c) - \frac{1}{\beta} S(c) ,$$

where β is the annealing parameter.

It can be proven that for fixed β and h , the minimization of the free energy leads to iterating over two steps

$$\mathbb{P}(x_i \in C_k) = \frac{\exp(-\beta e_{ik})}{\sum_{j=1}^K \exp(-\beta e_{ij})}, \quad (6.3)$$

where $e_{ik} = \frac{1}{2} \sum_{j=1}^K h_{jk}(t) \|x_i - m_j(t)\|^2$ and

$$m_k(t+1) = \frac{\sum_{i=1}^N x_i \sum_{j=1}^K h_{jk}(t) \mathbb{P}(x_i \in C_j)}{\sum_{i=1}^N \sum_{j=1}^K h_{jk}(t) \mathbb{P}(x_i \in C_j)}. \quad (6.4)$$

If $\beta \approx 0$, there is only one global minimum computed by a gradient descent or EM schemes. When $\beta \rightarrow +\infty$, the free energy tends to be $E(m, c)$, the classical batch SOM is retrieved and most of the local minima are avoided. The deterministic annealing minimizes the free energy, starting from a small β , to finally get (with increasing β) an approximation of the global minimum of $E(m, c)$.

6.3. Probabilistic models

Other variants of SOM use a probabilistic framework. The central idea of those approaches is to constrain a mixture of Gaussian distributions in a way that mimics the SOM grid.

Consider a mixture of K Gaussian distributions, centered on the prototypes, with equal covariance matrix,

- In the *Regularized EM* [35], the constraint is enforced by a regularization term on the data space distribution;
- In the *Variational EM*, [61], the constraint is induced at the latent variable level (via approximating the posterior distribution of the hidden variables knowing the data points $p(Z|X, \Theta)$, where Θ is the parameter vector, by a smooth distribution);
- In the *Generative Topographic Mapping*, the constraint is induced on the data space distribution, because the centers of the Gaussian distributions are obtained by mapping a fixed grid to the data space via a nonlinear smooth mapping.

One can find more details about these SOM variants in the WSOM 2016 Proceedings [18]. All the probabilistic variants enable missing data analysis and easy extensions to non numerical data.

7. SOM FOR NON NUMERICAL DATA

The original definition of SOM was conceived to deal with vector numerical variables. Quickly, Teuvo Kohonen and other researchers[41], [43], [36], [38], [45], [48], [46], [47], [17] have proposed adaptations of SOM to categorical variables as those collected in surveys and for text mining.

SOM algorithm may be adapted to :

- Categorical data, like survey data, where the variables are answers to questions with multiple choices, or counting tables, where items are classified according to multiple criteria;
- Data described by a dissimilarity matrix or a kernel, where the observations are known by their pairwise relations. This framework is well adapted to data like graphs, categorical time series, etc.

7.1. Contingency data

The adaptation of the SOM algorithm to contingency data (named KORRESP) was first defined by Cottrell et al. in 1993 [16]. The data consists in a contingency table which crosses two categorical variables and which is denoted by $\mathbf{T} = (t_{i,j})$ with I rows and J columns. The idea is to mimic the Factorial Correspondence Analysis, which consists in two simultaneous weighted Principal Component Analysis of the table and of its transposed, using the χ^2 distance instead of the Euclidean distance. Therefore, to be able to take into account the χ^2 distance and the weighting, to comply with the way it is defined in the Multiple Correspondence Analysis. After transforming the data, two coupled SOMs using the rows and the columns of the transformed table can thus be trained. In the final map, related categories belong to the same cluster or to neighboring clusters. The reader interested in a detailed explanation of the algorithm can refer to [4]. More details and real-world examples can also be found in [11, 13]. Note that the transformed tables are numerical data tables, so there is no particular theoretical results to comment on. All the results that we presented for numerical data still hold.

So the algorithm KORRESP can be defined in three steps:

- First, scale the rows and the columns as in Factorial Correspondence Analysis and replace the table T by

the scaled contingency table denoted by T^{sc} , where

$$t_{i,j}^{sc} = \frac{t_{i,j}}{\sqrt{t_i \cdot t_j}}$$

with $t_i = \sum_j t_{ij}$ and $t_j = \sum_i t_{ij}$;

- Then build an extended data table X by associating to each row, the most probable column and to each column, the most probable row;
- Finally, simultaneously classify the rows and the columns onto a Kohonen map, by using the extended data table X as input for the SOM algorithm.

The approach is summarized in the scheme Figure 8.

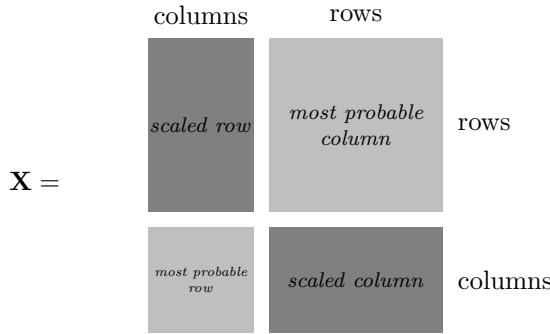


Figure 8: The extended data table X

Note that the assignment step uses the scaled rows or columns, the prototype update concerns the extended rows or columns and that the same are alternatively drawn at random. After convergence, rows and columns items are simultaneously classified as in FCA, but on one map only. In real world applications, the data can be collected in surveys or text mining and can be more complex than a simple contingency table crossing two questions. They can be collected as a Burt Table, i.e. a

full contingency table for more than two questions or a complete disjunctive table that contains the answers of all the surveyed individuals. KORRESP deals with all these kinds of tables. It is sufficient to consider these tables as “contingency tables” crossing their rows and their columns.

Let us take a simple example to illustrate the KORRESP algorithm. Table 2 displays the distribution of the 12,585 monuments listed in France in 1990, according to their category (11 levels) and their owners (6 levels) [16]. We use a KORRESP algorithm to simultaneously cluster the categories of monuments and their owners on a 5×5 Kohonen map.

Monument	Town (TO ₋)	Private (PR ₋)	State (ST ₋)	Department (DE ₋)	Public Establishment) (PU ₋)	Other (OT ₋)
Prehistoric antiquities (PRE)	244	790	115	9	12	144
Historical antiquities (HIS)	246	166	46	23	11	31
Castles and manors (CAS)	289	964	82	58	40	2
Military architecture (MIL)	351	76	59	7	2	0
Cathedrals (CAT)	0	0	87	0	0	0
Churches (CHU)	4298	74	16	5	4	2
Chapels and oratories (CHA)	481	119	13	7	8	4
Monasteries (MON)	243	233	44	37	18	0
Public secular monuments (PUB)	339	47	92	19	41	2
Private secular monuments (PRI)	224	909	46	7	18	4
Others (OTM)	967	242	109	40	10	9

Table 2: Historical monuments classified by category and kind of owners, 1990, France, Source MCC/DPVDEP

Table 3 presents the resulting Kohonen map after learning, which shows the main associations between monument categories, between owners types, between monument categories and owner types. One can see, for example, that the cathedrals (CAT) and the state (ST₋) are in the same cluster, as foreseen since the cathedrals in France belong to the State. Similarly, the castles (CAS), the private secular monuments (PRI) are with the Owner Private (PR₋). The churches and the chapels belong to the towns in France and, as expected, are close to the owner Town (TO₋).

The Kohonen map gives interesting information on these associations, in line with the results obtained by using a Factorial Correspondence Analysis, on one map only, while many projections are required to correctly interpret the results of a Factorial Analysis.

PRE OT_-	HIS	MIL OTM		CHU
		CHA	TO_-	
CAS PRI PR_-				
MON DE_- PU_-		PUB		CAT ST_-

Table 3: The monuments, their categories and their owners on the Kohonen map

7.2. Median SOM

When the data are known only through relational measures of resemblance or dissemblance, such as kernels or dissimilarity matrices, it is also possible to extend the original SOM algorithm. Both on-line and batch versions were proposed during the last two decades. These versions can be used for data-like graphs (social networks) or sequences (DNA sequences) for example. A detailed review of these algorithms is available in [58].

The data is supposed to be described by a symmetric (dis)similarity matrix $\mathbf{D} = (\delta(x_i, x_j))_{i,j=1,\dots,N}$, in a discrete setting. Note that observations (x_i) do not necessarily belong to a vector space.

One of the first attempts was proposed by Kohonen and Somervuo, 1998, [38], and is the Median SOM. The prototypes have to be equal to an observation. The optimal prototypes are computed by searching through $(x_i)_{i=1,\dots,N}$, instead of \mathcal{X} , as in [38], [48], [20], [21].

The Median SOM algorithm is defined by a discrete optimization scheme, in a batch mode:

1. Assignment of all data to their best matching units: $c^t(x_i) = \arg \min_k \delta(x_i, m_k(t))$;
2. Update of all the prototypes within the dataset by $m_k(t) = \arg \min_{x_i} \sum_{j=1}^N h_{c^t(x_j)k}(t) \delta(x_i, x_j)$.

As the algorithm explores a finite set, it is convergent to a local minimum of the energy function. But there are some drawbacks: all prototypes must belong to the data set, and the induced computational cost is very high.

7.3. Relational SOM

Another class of algorithms well adapted to data known by a dissimilarity matrix relies upon a result obtained by Goldfarb, 1984 [30], which shows that if the data is described by a (dis)similarity matrix $\mathbf{D} = (\delta(x_i, x_j))_{i,j=1,\dots,n}$, they can be embedded in a pseudo-Euclidean space:

Theorem 7.1. *There exist two Euclidean spaces \mathcal{E}_1 and \mathcal{E}_2 and $\psi_1 : \{x_i\} \rightarrow \mathcal{E}_1$, $\psi_2 : \{x_i\} \rightarrow \mathcal{E}_2$ such that*

$$\delta(x_i, x_j) = \|\psi_1(x_i) - \psi_1(x_j)\|_{\mathcal{E}_1}^2 - \|\psi_2(x_i) - \psi_2(x_j)\|_{\mathcal{E}_2}^2.$$

The principle of the adapted algorithm is to use the data representation in $\mathcal{E} = \mathcal{E}_1 \otimes \mathcal{E}_2$, where $\psi(x) = (\psi_1(x), \psi_2(x))$.

- The prototypes are expressed as convex combinations of the $(\psi(x_i))$:

$$m_k(t) = \sum_{i=1}^N \gamma_{ki}^t \psi(x_i)$$

where $\gamma_{ki}^t \geq 0$ and $\sum_i \gamma_{ki}^t = 1$;

- The distance $\|\psi(x_i) - m_k(t)\|_{\mathcal{E}}^2$ can be expressed with \mathbf{D} and the γ by

$$(\mathbf{D}\gamma_k^t)_i - \frac{1}{2}(\gamma_k^t)^T \mathbf{D}\gamma_k^t.$$

where $(\gamma_k^t)^T = (\gamma_{k,1}^t, \dots, \gamma_{k,N}^t)$.

Then the first step of the algorithm, finding the best matching unit of an observation, as introduced in Equation (2.1), can be directly generalized to dissimilarities, *both for on-line and batch settings*. As for the prototype update, it should be noted that it only concerns the coordinates (γ_k) . For the *on-line framework* [54], it is written as in the original SOM, (see Equation (2.2)):

$$\gamma_k^{t+1} = \gamma_k^t + \varepsilon(t) h_{kc^t(x_i)}(t) (\mathbf{1}_i - \gamma_k^t) \quad (7.1)$$

where x_i is the current observation and $\mathbf{1}_{il} = 1$ if $l = i$ and 0 otherwise.

In the *batch framework* [33], [32], the prototypes update is identical to the original Batch algorithm (see Equation (5.2)). One puts

$$m_k(t+1) = \sum_{i=1}^N \frac{h_{kc^t(x_i)}(t)}{\sum_{j=1}^N h_{kc^t(x_j)}(t)} \psi(x_i) \Leftrightarrow \gamma_k^{t+1} = \frac{h_{kc^t(x_i)}(t)}{\sum_{j=1}^N h_{kc^t(x_j)}(t)}. \quad (7.2)$$

If the dissimilarities are in fact given by Euclidean distances between data points in \mathbb{R}^p , the relational SOM is strictly equivalent to the original SOM.

7.4. Kernel SOM

A kernel $\mathbf{K} = (K(x_i, x_j))_{i,j=1,\dots,N}$ is a particular case of symmetric similarity measure, positive semi-defined and satisfying

$$\forall M > 0, \forall (x_i)_{i=1,\dots,M} \in \mathcal{X}, \forall (\alpha_i)_{i=1,\dots,M}, \sum_{i,j} \alpha_i \alpha_j K(x_i, x_j) \geq 0.$$

Observe that a kernel matrix \mathbf{K} is a Euclidean dot product, but that a dissimilarity matrix \mathbf{D} may not necessarily be transformed into a kernel matrix. For kernel data, Aronszajn, 1950, [1] proves the following result:

Theorem 7.2. *There exists a Hilbert space \mathcal{H} , also called feature space, and a mapping $\psi : \mathcal{X} \rightarrow \mathcal{H}$, called feature map, such that $K(x_i, x_j) = \langle \psi(x_i), \psi(x_j) \rangle_{\mathcal{H}}$ (dot product in \mathcal{H}).*

The SOM algorithm can be extended to kernel SOM (see [62], [50]), following the steps mentioned below:

- The prototypes are expressed as convex combinations of the $(\psi(x_i))$:

$$m_k(t) = \sum_{i=1}^N \gamma_{ki}^t \psi(x_i)$$

where $\gamma_{ki}^t \geq 0$ and $\sum_i \gamma_{ki}^t = 1$;

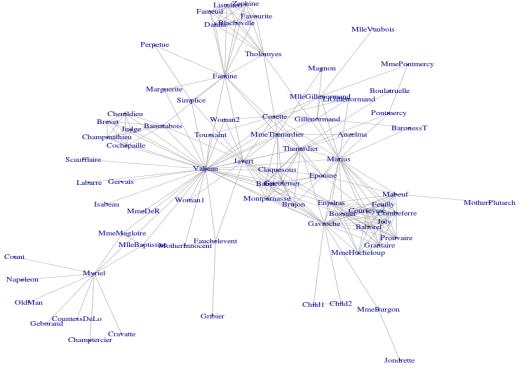


Figure 9: Graph of co-occurrences for the characters in the Misérables

- The distance is given by

$$\|\psi(x_i) - m_k(t)\|^2 = (\gamma_k^t)^T \mathbf{K} \gamma_k^t - 2\mathbf{K}_i \gamma_k^t + \mathbf{K}_{ii},$$

where \mathbf{K}_i is the i th row of \mathbf{K} and $(\gamma_k^t)^T = (\gamma_{k,1}^t, \dots, \gamma_{k,N}^t)$.

The prototype updates are the same as before, acting only on the γ . Note that if the dissimilarity is the squared distance induced in the feature space \mathcal{H} , kernel SOM and relational SOM are strictly equivalent.

The algorithms are fully equivalent to the original SOM algorithms for numerical data in the feature (implicit) Euclidean space induced by the dissimilarity or the kernel, as long as the prototypes are initialized in the convex hull of the input data. So the relational/kernel versions suffer from the same theoretical limitations as the original SOM algorithms.

7.5. Example: The characters in "Les misérables"

This example is extracted from the paper by Olteanu and Villa, 2015, [55]. Let us define the graph of co-occurrences (in the same chapter) of the 77 characters in the Victor Hugo's novel “Les misérables”. It is displayed in Figure 9.

The dissimilarity between two characters is defined as the length of the shortest path between two vertices. The resulting Kohonen map using the relational on-line version is displayed in Figure 10.

A hierarchical clustering of the prototypes is used to build “super-classes”, which are displayed in Figure 11, where the size of the clusters is proportional to the number of characters.

In Figure 12, one can color the characters in the initial graph with the color of the super-classes.

Figure 13 presents a simplified graph, built from the super-classes. Each super-class is represented by a circle with a radius proportional to the number of vertices it contains. The width of the edges is proportional to the number of connections between two super-classes.

7.6. Example: Professional trajectories

The data comes from a project “Generation 98 à 7 ans”, 2005, of CERÉQ, Centre Maurice Halbwachs (CMH), France. To collect the data, 16,040 young people leaving initial training in 1998 are observed over 94 months. Each month, the nature of their activity is recorded (permanent labor contracts,

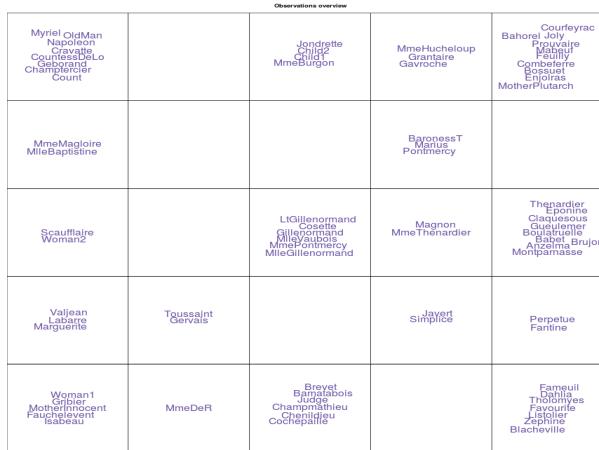


Figure 10: The Kohonen map

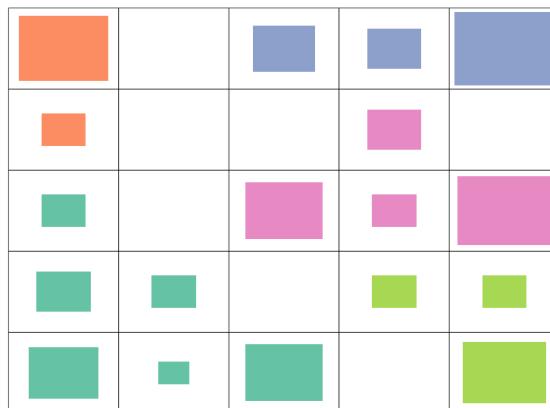


Figure 11: Super-classes of characters

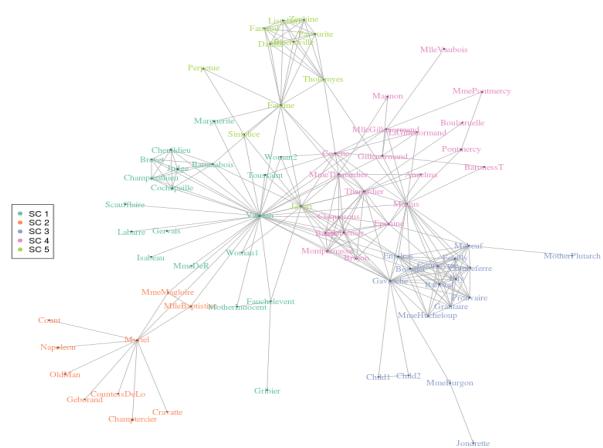


Figure 12: The colored graph

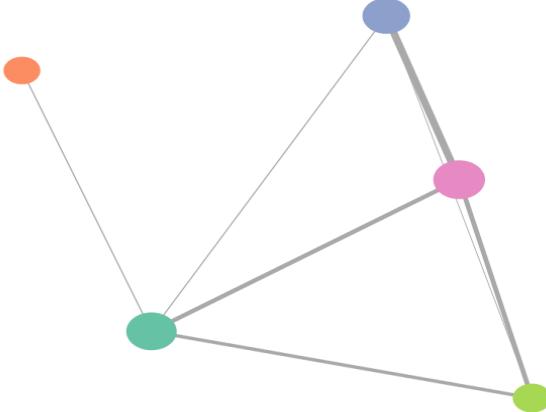


Figure 13: The simplified graph

fixed-term contracts, apprenticeship program, public temporary-labor contract, on-call contract, unemployment, inactive, military service, education,...).

The dissimilarity between recorded sequences is defined as the Optimal Matching, which is a variant of the Edit Distance where some costs are assigned to the changes. After the relational SOM is trained on the entire data set, one gets the final map illustrated in Figure 14 [54].

8. CONCLUSION AND PERSPECTIVES

We have presented the original on-line and Batch SOM, as well as some of their variants. Although many practical evidences do not have rigorous mathematical proofs so far, these algorithms are widely used to solve a large range of problems. The extensions to categorical data, dissimilarity data, kernel data have transformed them into even more powerful tools. Since the Heskes's variants of SOM have a more solid theoretical background, SOM can appear as an easy-to-develop approximation of these well-founded algorithms. This observation should ease the concern that one might experience about it.

Their non supervised learning characteristic makes them very interesting to use for exploratory data analysis, as there is no need to be aware of the labels. The fact that the algorithm complexity is linear with respect to the database size makes them very well adapted to Big Data problems. Another useful property of SOM algorithm is its ability to deal in a straightforward way with databases containing some missing data, even if they are numerous, see [14].

To conclude, let us emphasize an aspect which has yet to be deeply exploited. Mostly in practical applications, the stochasticity of the results is viewed as a drawback, since different runs of the on-line SOM provide different resulting maps. For that reason, some people preferentially use the Batch version of SOM.

In fact, this stochasticity can be very useful in improving the performances and more precisely qualifying the results. Three lines of inquiry seem promising:

- It allows to improve the stability as shown in the following papers [56, 59, 63, 2, 51, 52];
- This stochasticity can be used to qualify the reliability of the results with a stability index [19];
- Or to distinguish stable pairs and fickle pairs of data points to improve the interpretation and the visualization as in [4] and [5] for medieval text mining.

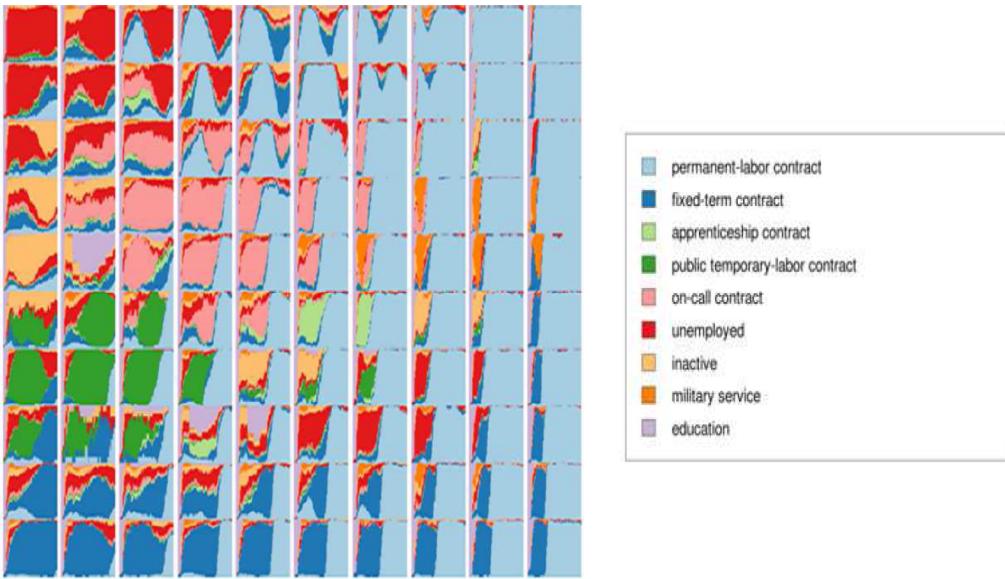


Figure 14: Top left: exclusion of the labor market. Top right: quick integration

Note that Batch SOM for numerical data or relational data is implemented in the **R**-package **yasomi** (<http://yasomi.r-forge.r-project.org>), and that KORRESP and on-line SOM for numerical data or relational data are implemented in the **R**-package **SOMbrero** (<https://CRAN.R-project.org/package=SOMbrero>).

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