

# Polymorphic Self-Organizing Maps framework

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**Abstract** Self-organizing maps (SOM) are widely used to classify vectorial data. However, its methodology is not restricted to metric vector spaces. In this paper we introduces a self-organized map framework to classify any kind of data with only two restrictions: namely, the existence of a distance measure for input elements, and the possibility to interpolate a new element between other two with a certain distance. We formilizes the requiriments to define a distance measure and the interpolation functions and, as a practical example, following this philosophy we implemented a SOM for symbol strings.

**Keywords** Self-organizing maps; Framework; Clustering; Visualization; Data mining; Nonvectorial data

## 1 Introduction

Self-Organizing Maps (SOM) (Tuevo Kohonen [4,5]) are widely used for unsupervised learning, clustering, classification, and visualization of any kind of data. More than

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5000 publications [?] can be found in the literature in the last years. Many of these works propose significant approaches to deal with vectorial data. The use of linear vector spaces in SOM decrease the complexity thanks to the Euclidean distance and to the arithmetical operations usually implemented as basic instructions in computer processors. These special characteristics of numerical vectors makes easy to implement fast SOM algorithms. However, areas with increasing relevance like image processing, bioinformatics, or speech recognition need to deal with nonvectorial data.

There are two approaches to work in SOM with nonvectorial data. One approach consist on transforming input data to vectorial one. The other approach, is based on SOM algorithm modification to enable it to deal directly with a certain data type. Codify input data as numerical vectors, usually require high efforts for analysis and implementation. Sometimes, this transformation is not possible or reduce certain characteristics of original data. In a recent published work [?] we made clustering and visualization of HIV Quasiespecies using SOM. In this paper we have codified original ARN sequences to vectors using *Hamming* distance finding some inconveniences in this process. That experience gided as to work with the second approach.

A good methodology to deal with nonvectorial data directly, is described by T. Kohonen and P. Somervuo in [6]. This method modify original SOM algorithm calculating a *Median Set* as model. Studies over the median for symbol strings in [?] demonstrates the NP-Complete complexity. That inconvenience joint with the loss of graduality in learning process motivate us to search for a new methodology that will be nearer to the original SOM simplicity and elegance. In this way, we developed a method that start with SOM for vectorial data algorithm making minimum changes. We have been analized the algorithm in order to identify the steps that modify the models. In original SOM for vectors, the models has same type than input data. Once, we located these crucial steps, we modify it to make it more general. The idea is to provide the needed elements that permit us to work with any type of data. The *model updating process* is one of these steps that "touch" directly the input data. Other operation like calculating neighborhood depends on data coordinates in the grid and not on data itself.

In this paper we propose a framework for SOM that permit us to deal with any kind of data maintaining original vectorial SOM concepts and we formalizes the requirements to implement new modules for any input data type. As example we have implemented the AI::NeuralNet::SOMString Perl module. We present in Sec. ?? some results for strings clustering experiments.

The paper is organized as follows: Sec. ?? contains a brief survey of works related to the application of SOM to nonvectorial data. Sec. 4 introduces our new algorithm based on the use of discrete entities interpolation. Sec. 6 is devoted to describe two experemental examples in order to study how our proposal works with symbol strings and the perfomance of our method method with large data sets.

## 2 State of the art

Tengo que hablar de trabajos relacionados. Cosas que tengo que contar: - The batch map for strings: "Sammon" projection?

The Self-Organizing Map (SOM) was introduced by Teuvo Kohonen in 1982 (see [4,5] for details).

Learning Vector Quantization (LVQ) supervised learning. No neighborhood are defined around the winner. LVQ can be used to fine tuning the SOM reference vectors for best class separations [7]

To deal with nonvectorial data, there are two approaches. One of them approaches is based on codify input data with real vectors. There are good examples of this method in [1, ?, 10]. Other approach is based on create a map of models using directly original data. Changes in SOM algorithm are made to make it capable to deal directly with non vectorial data. One of these methods is *Median SOM* described originally in [2] and Kohonen and Somervuo in [6] have shown how this algorithm works for clustering a large protein sequence database. We will describe it in section ?? describes this method. We find *Median SOM* examples in [?]. We propose a new simple method that no changes on input data are needed. Will be possible to re-use early all the original implementation and need only to include two new functions *integer distance(elementA, elementB)* and *element interpolateNewElement(distance, sourceElement, targetElement)*. Section ?? describe this two new functions.

An implementation of multidimensional vectorial SOM developed by T.Kohonen is available in [?]. After the seminal Kohonen works, several works have been published that try to enhance the original SOM implementation. Examples of these works are [8, 9], and [3] where the authors use evolutionary-learning to make a faster SOM implementation without using a distance function.

### 3 Self-Organizing Map

The SOM is a non-supervised neural network that tries to imitate the self-organization done in the sensory cortex of the human brain, where neighbouring neurons are activated by similar stimulus. It is usually employed either as a clustering/classification tool or as a method to find unknown relationships among a set of variables that describe a problem.

The main property of the SOM is that it makes a nonlinear projection from a high-dimensional data space (one dimension per variable) on a regular, low-dimensional (usually 2D) grid of neurons (see Figure ??), and, from the self-organization process, the projection preserves the topologic relations while simultaneously creating a dimensional reduction of the representation space (the transformation is made in a topologically ordered way).

The SOM processes a set of input vectors (samples or patterns), which are composed by variables (features) typifying each sample. It then creates an output topological network where each neuron is also associated to a vector of variables (model vector) which is representative of a group of the input vectors. Note in Figure ?? that each neuron of the network is completely connected to all the nodes (each node is a sample) of the input layer. So, the network represents a feed-forward structure with only one computational layer formed by neurons or model vectors.

There are four main steps in the processing of the SOM. Except the first one, the others are repeated until a stop criterion is met:

- **Initialization of model vectors.** Usually it is made by assigning small random values to their variables, but there are some other possibilities such as an initialization using random input samples.

- **Competitive process.** For each input pattern  $X$ , all the neurons (model vectors)  $V$  compete using a *similarity function* in order to identify the one most similar or closest to the sample vector. Usually, the similarity function is a distance measure (such as an Euclidean distance). The winner neuron is called the best matching unit (BMU).
- **Cooperative process.** The BMU determines the centre of a topological neighbourhood where those neurons inside it (the model vectors) will be updated to be even more similar to the input pattern. A *neighbourhood function* is used to determine the neurons to consider. If the lattice where the neurons are is rectangular or hexagonal, it is possible to consider as neighbourhood functions rectangles or hexagons with the BMU as centre. However, it is more usual to use a Gaussian function to assure that the farther the neighbour neuron is, the smaller the updating to its associated vector is. In this process, all the neurons within a vicinity cooperate to learn.
- **Learning process.** In this step the variables of the model vectors within the neighbourhood are updated to be closer to those of the input vector. It means making the neuron more similar to the sample. The *learning rule* used to update the vector ( $V$ ) for every neuron  $i$  in the neighbourhood of the BMU is:

$$V_i^t = V_i^{t-1} + \alpha^t \cdot N_{BMU}^t(i) \cdot (X - V_i^{t-1}) \quad (1)$$

Where  $t$  is the current iteration of the whole process,  $X$  is the input vector,  $N_{BMU}$  is the neighbourhood function for the BMU, which returns a high value (in  $[0,1]$ ) if the neuron  $i$  is in the neighbourhood and close to the BMU (1 if  $i = BMU$ ), and a small value otherwise (0 if  $i$  is not located inside the neighbourhood); and  $\alpha$  is the *learning rate* (in  $(0,1]$ ). Both neighbourhood and learning rate depend on  $t$ , since it is usual to decrease the radius of the first one and the value of the second in order to impose a higher updating rate at the beginning of the process and almost none in the final iterations.

The recurrent application of Equation 1 and the update of the neighbourhood function, has the effect of ‘moving’ the model vectors,  $V_j$  from the winning neuron towards the input vector  $X_i$ . That is, the model vectors tend to follow the distribution of the input vectors. Consequently, the algorithm leads to a topological arrangement of the characteristic map of the input space, in the sense that adjacent neurons in the network tend to have similar weights vectors.

The SOM is further processed using Ultsch method [?], the Unified distance matrix (U-Matrix). It uses SOM’s codevectors (vectors of variables of the problem) as data source and generates a matrix where each component is a distance measure between two adjacent neurons.

The U-Matrix shows a lattice where there are one cell per neuron in the map, which is the best matching unit for one (or more) of the input samples, and one more cell between every pair of neurons, which represents the distance between them. This distance is showed using a color code (usually blue means near or little distance, and red far or large distance). Each cell corresponding to one neuron in the map may be labeled with the related tag of the pattern which it represents.

It allows us to visualize any multi-variates dataset in a two-dimensional display, so we can detect topological relations among neurons and infer about the input data structure. High values in the U-matrix represent a frontier region between clusters, and

**Fig. 1** Left: SOM with 20 neurons (4 rows and 5 columns) and marked neighborhood area with radius 1, centered in winner neuron in a rectangular topology. Right: graphical representation of SOM training process

low values represent a high degree of similarities among neurons on that region, i.e. clusters.

Therefore, looking at the output of a SOM and its corresponding U-Matrix, it is possible to recognize some clusters as well as the metric-topological relations of the data items (vectors of variables of the problem) and the outstanding variables.

Although Kohonen's SOMs are not as accurate as other tools at the task of classification, they can be applied to many different types of data, yielding a visualization of natural structures in the data and their relations, as well as the natural groupings that could be among them. In addition, SOMs make easy the estimation of the variables that have more influence on these groupings, via the so-called planes analysis. Other statistical and soft computing tools can also be used for this purpose, but Kohonen's SOMs offer a visual way of doing it which is much more intuitive.

## 4 A generalized SOM approach for any kind of data

### 4.1 The SOM approach for vectorial data

SOM learning process iteratively performs the following three steps:

- A certain element of input data is chosen.
- The model of the SOM grid with the best matching with the selected datum is located
- This winner model and its neighborhood is appropriately updated

In this process, the distance measure plays a significant role: the winner model is the *closest* one to the input datum and the update is carried out with the aim of taking the neighborhood *nearer* to the input datum (see Fig. 2). In the case of vectorial data, for each model  $m_i$ , the following formula is used to calculate the updated value:

$$m_i(t+1) = m_i(t) + h_{ci}(t)[x(t) - m_i(t)] \quad (2)$$

where  $m_i(t)$  is the model located at  $i$  grid position,  $x(t)$  is the selected input datum,  $t = 0, 1, 2, \dots$  is the discrete-time coordinate, and  $h_{ci}(t)$  is called *neighborhood function*. This *neighborhood function* usually takes a *Gaussian* form:

$$h_{ci}(t) = \alpha(t) \cdot \exp\left(-\frac{\|r_c - r_i\|^2}{2\sigma^2(t)}\right) \quad (3)$$

where  $\alpha(t)$  is the learning factor in time  $t$ ,  $r_c$  and  $r_i$  are the locations of models  $c$  and  $i$  respectively, and  $\sigma(t)$  stands for the Gaussian width.

[include Gaussian function graphic]

The goal of this equation is to compute a new value  $m_i(t+1)$  which is  $h_{ci}(t)[x(t) - m_i(t)]$  nearer to  $x(t)$  and  $h_{ci}(t)[x(t) - m_i(t)]$  farther from  $m_i(t)$ . With vectorial data the "+" operator together with the euclidean distance permits us to easily obtain the new value. However, if we are working with nonvectorial data this process has to be appropriately adapted.

#### 4.2 Working with any kind of data

If we want to apply the above described process to nonvectorial data, we need to find a suitable distance measure and an operator that allows us to take the models closer to the selected input datum at each iteration. Let us formalize this idea.

**Theorem 1 (Conditions for distance function)** *Let  $D$  be a data domain (vectorial or not). Let  $d : D \times D \rightarrow R$  be a distance function denoted  $d(x,y)$ . The distance function must hold the following conditions for each pairs of elements  $x, y \in D$ :*

- C1)  $d(x, y) \geq 0$  where equality holds if and only if  $x = y$ .*
- C2)  $d(x, y) = d(y, x)$*
- C3)  $d(x, y) \leq d(x, z) + d(z, y)$*

**Theorem 2 (Neighbor Data Set)** *Let  $D$  be a data domain. Let  $d : D \times D \rightarrow R$  be a distance function with the above Theorem restrictions. The Neighbor Data Set of distance  $\delta$  of value  $x$ ,  $N(x, \delta)$ , is defined as follows:*

$$N(x, \delta) = \{y \in D | d(x, y) = \delta\}$$

That is, the Neighbor Data Set contains all the elements of domain  $D$  that are at distance  $\delta$  from a given datum  $x$ . With this definition, we can now proceed to define the operation that allows us to take a model closer to a given element of the domain.

**Theorem 3 (Interpolation function)** *Let  $D$  be a data domain (vectorial or not). let  $d : D \times D \rightarrow R$  be a distance function. We say that  $I : D \times D \times R \rightarrow D$  is an Interpolation function if the following property holds:*

$$I(x, y, \delta) \in N(x, \delta) \cap N(y, d(x, y) - \delta), \forall \delta \leq d(x, y)$$

That is, the interpolation function, given two elements  $x$  and  $y$  of the domain and a distance  $\delta$ , permits us to obtain a new element  $I(x, y, \delta)$  that is  $\delta$  farther from  $x$  and  $\delta$  closer to  $y$ . In the case of our SOM grid, the interpolation function permits us to generalize equation 2 as follows:

$$m_i(t+1) = I(m_i(t), x(t), h_{ci}(t) \cdot d(m_i(t), x(t))) \quad (4)$$

This way, with the generalized versions of the + operator and the euclidean distance, we can now apply the above method to any kind of data with the only restriction of having both a suitable distance and interpolation functions.

**Fig. 2** Updating a SOM with symbol string models using interpolation:  $x(t) = ABCD$  and  $m_i(t) = A$ . The new interpolated valued with, e.g.,  $h_{ci}(t) = 1$  is  $m_i(t+1) = AB$ . Only one change that leave  $m_i(t+1)$  nearest to  $x(t)$ . Left: before model updating, Right: After model updating.

#### 4.3 The extended algorithm

### 5 The case of strings

#### 5.1 A distance measure for string data

**Hamming Distance** Originally this distance measure was defined for binary codes but can be applied to any ordered set of discrete values. The hamming distance is defined only for strings of equal length. The distance consist of the number of different symbols.

```
x = (1,0,1,1,1)
y = (0,1,1,0,1)
dH(x,y)=3
```

```
u=(s,a,l,e)
v=(y,a,l,e)
dH(u,v)=1
```

**Levenshtein or Edit distance** The distance between strings A and B is defined as:

$$LD(A, B) = \min\{a(i) + b(i) + c(i)\} \quad (5)$$

B is obtained from A by a(i) replacements, b(i) insertions and c(i) deletions of a symbol. There exist an infinite number of combinations for  $\{a(i) + b(i) + c(i)\}$ , but the minimum can be formed using a dynamic-programming method. The distance measure is more reliable if the editing operations are provided with different weights. There are a weighted version of Levenshtein distance described by T. Okuda et al. in [?], with this equation:

$$WLD(A, B) = \min\{pa(i) + qb(i) + rc(i)\} \quad (6)$$

where  $p$ ,  $q$  and  $r$  may be obtained from the confusion-matrix of the alphabet, as the inverse probabilities for particular types of error to occur. However, this is only usefull for strings of words.

**String::Diff algorithm distance** This distance measure is based on String::Diff Perl module developed by Kazuhiro Osawa. It is similar to Levenshtein distance, but without using replacements as a basic edit operation.

The distance between strings A and B is defined as:

$$SDD(A, B) = \min\{b(i) + c(i)\} \quad (7)$$

B is obtained from A by b(i) insertions and c(i) deletions of a symbol

To compute string distance we use String::Diff Perl module. This is a fast algorithm to obtain strings differences. This is a execution example of String::Diff module wrote in Perl:

```
my $diff = String::Diff::diff_merge("AB", "ABCDE",
    remove_open => "<del>",
    remove_close => "</del>",
    append_open => "<ins>",
    append_close => "</ins>",
);
print "$diff\n";# this is AB<ins>CDE</ins>
```

Arguments *remove\_open*, *remove\_close*, *append\_open* and *append\_close* indicates the marks for insert or delete a substring. We have transformed original String::Diff output, to this one:

```
#This is new diff string AB<ins>C</ins><ins>D</ins><ins>E</ins>
```

It is easy to interpolate a new symbol string with a certain distance using this difference string.

## 5.2 An interpolation function for string data

***new\_interpolated\_model implementation for symbol strings*** Other important element required to compute new SOM algorithm for nonvectorial data is *new\_interpolated\_model* function. We have to implement a different function for each data type we want to compute. In case of symbol strings we implemented two different version. One of this is based on Levenshtein algorithm. This version has complexity  $O(n^3)$ . When string lengths is more than 1000 characters as will be the case of DNA strings, SOM algorithm time to compute increase drastically. This is the reason why we test different distances measures and finally decided to use String::Diff package. This implementation is fast for any string length. Other advantage this measure has got is the possibility to easily interpolate new string using difference string output. This is the pseudocode for *new\_interpolated\_model* function:

```
new_interpolated_model( $m_i(t)$ ,  $x(t)$ ,  $d(t)$ ) {
    diff = distance( $m_i(t)$ ,  $x(t)$ )
    return calculate_new_model(diff,  $d(t)$ )
}
```

where *calculate\_new\_model(diff, d(t))* function, process the difference string returned by *distance( $m_i(t)$ ,  $x(t)$ )* function doing *d(t)* number of changes. Let the difference string returned by distance function:

```
AB<ins>C</ins><ins>D</ins><ins>E</ins>
```

make *d(t)* changes over it, will result the string:

```
ABCD<ins>E</ins>
```

to obtain the new interpolated string the only thing needed is to eliminate the substring starting at first "ins" or "del" and finishing at string end. In this example, new interpolated string will be "ABCD". The string have distance 2 from "AB" and is two positions nearer to "ABCDE"



**Fig. 3** Symbol string clustering 10x10 SOM after training process. Input data set consist of five strings: CAT, CATTLE, BAT, BATTLE and BATTLEFIELD.

### 5.3 The approach for string

## 6 Experimentation

We included in this paper two experiments to illustrate how the algorithm works. First one, are developed using a short symbol string data set in order to easily check clustering capabilities. The second one, is made using a database with 100.000 english word to test how the algorithm works with a large database.

To test the new algorithm presented in Sec. 4 we have implemented a new Perl module called `AI::NeuralNet::SOMString`. This Perl module is based on a previous implementation developed by Alexander Voischev called of `AI::NeuralNet::SOM`. One element required to SOM implementation is a distance measure. There are several options to calculate a symbol string distance. We presents some of the most used symbol string distances.

**Input selection** An important aspect in SOM experiments is how input are ordered. If we have, e.g., an alphabetically ordered english dictionary as input data set, with radius around 3, we can see the whole map first with words starting with "A", then with words starting with "B" and same with all letters in alphabet. Depending on when we decided to stop the learning process, the map will show a clustering view or other drastically different. Will be better to merge randomly the dataset before use it.

Table 1 represents SOM arguments for the experiment. Note that radius is nearest to SOM array dimension. Several experiments realized with smallest radius values, results in maps with no updated areas. Initial randomly used valued remain after training process. Gaussian Neighborhood function change deeply neurons that are closes to winner. Linear alpha function makes the transitions between clusters gradually. Fig. 3 resrepresents SOM for strings using a initialization map with string randomly generated with a length no longer than three characters. Fig. 4 represents umatrix for same SOM. Labels is umatrix is the result of map calibration. Taking each input value and locating in the map the nearest value. This map present several models with same distance to each input value. In this case we take one of them randomly.

### 6.1 Simple data set experiment

*Data set description* This experiment uses same dataset than Panu Somervuo in [11] to easily compare results. Data sets consist on five strings: CAT, CATTLE, BAT, BATTLE and BATTLEFIELD.

**Table 1** Arguments for SOM using short symbol string dataset

Argument	Value
Alpha	0.5
Radius	9.9
Neighborhood function	Gaussian
Alpha function	Linear
Rows	10
Columns	10
Rounds	27

**Fig. 4** 10x10 SOM umatrix representation. Input data set consist of five strings: CAT, CAT-TLE, BAT, BATTLE. and BATTLEFIELD. Black represent zero distance. Dark gray represents low distance and light gray represents high distance. This map is calibrated with input values. Each label is located in one of the best matching node.

## 6.2 Large database experiment

## 7 Conclusions and further work

Mathematical properties of discrete learning process like convergence, etc.

- Developed methods for winner selection

Observed differences between continuous data input and discrete data input:

1. **Shorter training process** than training process for real vectors. The number of possible changes are limited by the maximum distance between SOM models and input elements.
2. Depending on items distance and input data set diversity, after training, **SOM will present regions with zero distance**. This happens because possible values in training process are discrete and usually very short. In case of real values, after calculate a new  $model\ m_i(t+1) = m_i(t) + h_{ci}(t)[x(t) - m_i(t)]$  it is hard to have exactly the same values. Will be similar to use a discrete numerical space. Several input values will correspond to one output value, e.g., using a round function.
3. **Winner selection**. In case of real data, is difficult to have exactly the same distance after apply adapt function. In case of discrete values with a short range, it is easy to have several winners. In these cases, selection method for winners will be used. We used two methods for winner selection. First one, is a randomly selected winner from winner set. Experiments realized with this *winner selection method* for a large dataset cause no clustering, because each time a different area in map are selected for a certain model. [Sucesive] epochs will modify previous mini area and depending on radius will delete this mini area. Other method selection is to use first funded value. It is faster method and give good enough results. The reason why this method works is because first tends to be located always in same area and clustering is reinforced. When frontier values are selected to be updated, that updating process will not cause the deletion of a bigger cluster than in previous method. In a certain way, second one method (first winner) tends easily to clustering and first one (randomly winner selection) tends to dispersion.
4. In case of real values, it is easy to see map areas where there are no input elements coincidences. Thanks to Euclidean distance, after train process *models* are nearest

to the areas where impact more input values. I case of non numerical input values, is most difficult to see that. We have not a Euclidean distance that give as a spacial distance measure for the elements in the map. A way to know how many input values impact in any area we use a graphic with.

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