ABSTRACT

Controlling the internal representation space of a neural network is a desirable feature because it allows to generate new data in a supervised manner. In this paper we will show how this can be achieved while building a low-dimensional mapping of the input stream, by deriving a generalized algorithm starting from Self Organizing Maps (SOMs). SOMs are a kind of neural network which can be trained with unsupervised learning to produce a low-dimensional discretized mapping of the input space. They can be used for the generation of new data through backward propagation of interpolations made from the mapping grid. Unfortunately the final topology of the mapping space of a SOM is not known before learning, so interpolating new data in a supervised way is not an easy task. Here we will show a variation from the SOM algorithm consisting in constraining the update of prototypes so that it is also a function of the distance of its prototypes from extrinsically given targets in the mapping space. We will demonstrate how such variants, that we will call Supervised Topological Maps (STMs), allow for a supervised mapping where the position of internal representations in the mapping space is determined by the experimenter. Controlling the internal representation space in STMs reveals to be an easier task than what is currently done using other algorithms such as variational or adversarial autoencoders.

1 Introduction

Neural networks are a powerful tool because they can implement any kind of function by mapping the input space into an output domain with different dimensionality. This is done while extracting features from inputs so that the activity of deeper layers (far from the input layer) is an abstract representation of the more superficial ones. Nevertheless the way learning of the internal weights is achieved, makes them as black boxes and internal representations cannot be usefully deployed to build efficient and intuitive classifiers. Solving the issue of the intelligibility of internal representations requires two functionalities: first, the creation of internal representations must follow a meaningful heuristic; second, the position of representations in the layer must be known. Self organizing maps (SOMs – Kohonen [1982]) are a way to implement the first functionality. SOMs are competitive neural networks that allow for a low-dimensional discretized mapping of the input space. The training algorithm for SOMs is strictly related to the vanilla k-means clustering algorithm (MacQueen [1967], Bishop [2006]). We show here that both algorithm belong to a family of algorithms where each individual is defined by a different implementation of a winner-takes-all (WTA) operator which is a function of the distance between input patterns and prototypes, but can also depend on other variables, intrinsic or extrinsic w.r.t. the structure of the network. In particular we can define a variant whose WTA operator is also a function of the distance of prototypes from a desired point in the low-dimensional mapping space. We call This kind of network Supervised Topological Maps (STM). We show in this paper that controlling the internal representation space in STMs is easier than what can be currently done using other algorithms such as variational or adversarial autoencoders (Kingma and Welling [2013], Makhzani et al. [2015]). In the rest of the paper we will first describe the k-mean and SOM algorithms focusing on their strict relation (sections 2 and 3). Then we define STMs by describing their specific WTA operator (section 4). Finally we will show some examples of usage of STMs for the supervised generation of data (section 5) and we will discuss their relationship with other algorithms and their limitations (section 6).
2 k-means clustering

Vanilla k-means clustering divides the patterns of a dataset into $K$ clusters where $K$ is a fixed parameter. Each iteration of the algorithm is composed of two steps. In the first step input patterns are assigned to clusters based on their distance to the cluster centroids. Each pattern is assigned to its closer cluster. In the second step each $j^{th}$ centroid is substituted with the mean of all patterns belonging to the $j^{th}$ cluster.

Formally, the k-means algorithm can be described as a minimization over an energy function. Given a dataset $X = [x_1, \cdots, x_i, \cdots, x_N]^T \in \mathbb{R}^{N \times M}$, with each input pattern $x_i \in \mathbb{R}^M$, we can define the first step of the iteration as the application of WTA operator:

$$r_i = \arg \min_k ||x_i - c_k||$$

(1)

$$\phi_{i,j} = \begin{cases} 1 & \text{if } j = r_i \\ 0 & \text{otherwise} \end{cases}$$

(2)

and the definition the energy function based on the WTA operator:

$$L = \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{K} \phi_{i,j} ||x_i - c_j||^2$$

(3)

In the second step we minimize the energy function w.r.t each centroid $c_j$:

$$\frac{\partial L}{\partial c_j} = - \sum_{i=1}^{N} \sum_{j=1}^{K} \phi_{i,j} (x_i - c_j) = 0$$

(4)

$$c_j = \frac{\sum_{i=1}^{N} \phi_{i,j} x_i}{\sum_{i=1}^{N} \phi_{i,j}}$$

(5)

so that, as said before, each centroid $c_j$ is updated as the mean of all input patterns currently belonging to the $j^{th}$ cluster. The learning process ends when the centroids do not change anymore between iterations and the equilibrium is reached (see the full procedure in Algorithm 1).

The update step can be also applied iteratively:

$$c_j = c_j + \eta_i \phi_{i,j} (x_i - c_j)$$

(6)

where $\eta_i$ is the learning rate parameter, which is typically made to decrease monotonically as more data points are considered (Bishop, 2006). This iterative form highlights the strict relationship between k-means clustering and SOMs (see Algorithm 2 and Algorithm 4).

Algorithm 1: Vanilla k-means algorithm – batch version

**Input:** $X \in \mathbb{R}^{N, M}$: input dataset  
$C \in \mathbb{R}^{K, M}$: centroids of the $K$ clusters

**Output:**

while $\sum_{j=1}^{K} ||\Delta c_j|| < \epsilon$ do

\[ r_i = \arg \min_k ||x_i - c_k|| \]  // Index of the winner.

\[ \phi_{i,j} = \begin{cases} 1 & \text{if } j = r_i \\ 0 & \text{otherwise} \end{cases} \]  // Update operator.

\[ c_j = \frac{\sum_{i=1}^{N} \phi_{i,j} x_i}{\sum_{i=1}^{N} \phi_{i,j}} \]  // Updating of clusters.
Algorithm 2: Vanilla k-means algorithm – online version

Input: \( X \in \mathbb{R}^{N, M} \): input dataset
\( C \in \mathbb{R}^{K, M} \): centroids of the K clusters
\( \eta_{\text{init}} \): initial learning rate
\( \tau \): decay window
\( T \): number of epochs

for \( t \leftarrow 0 \) to \( T - 1 \) do
  \( \eta \leftarrow \eta_{\text{init}} e^{-\frac{t}{\tau}} \)
  shuffle \( X \)
  for \( i \leftarrow 1 \) to \( N \) do
    \( r_i = \arg \min_k ||x_i - c_k|| \)  // Index of the winner.
  for \( j \leftarrow 1 \) to \( K \) do
    \( \phi_{i,j} = \begin{cases} 1 & \text{if } j = r_i \\ 0 & \text{otherwise} \end{cases} \)  // Update operator.
    \( c_j \leftarrow c_j + \eta \phi_{i,j} (x_i - c_j) \)  // Updating of clusters.

3 Self Organizing Maps

SOMs are competitive neural networks, where competition between the units of the inner layer allows for the unsupervised emergence of a low-dimensional discretized map. One basic feature is that the inner layer has a predefined intrinsic topology, for instance, units in the inner layer can disposed in a 1-, 2- or 3-dimensional grid. After learning the weights of connections from the input layer to each unit in the inner layer become a prototype (centroid) of a cluster within the input dataset, in analogy with k-means cluster centroids. Similarly to k-means clustering, the update of centroids depends on a WTA competition based on the euclidean distance of input patterns from the centroids. Differently from k-means clustering the update also depends on the euclidean distance of the centroids from the winner centroid in the space of the inner layer. In particular, a radial-basis function of the euclidean distance from the winner in the inner layer space is used (will call it the neighboring function).

\[
    r_i = \arg \min_k ||x_i - w_k|| \quad \text{(7)}
\]
\[
    \phi_{i,j} = e^{-\frac{||j - r_i||^2}{2\sigma^2}} \quad \text{(8)}
\]

where \( W \in \mathbb{R}^{M \times K} \) is the matrix of weights, with each row being a prototype.

The learning process is commonly implemented as an online learning, where each input pattern presentation is followed by an update of the centroids.

\[
    w_j = w_j + \eta_i \phi_{i,j} (x_i - w_j) \quad \text{(9)}
\]

Since the update does not converge to equilibrium, the SOM algorithm needs annealing by letting both the learning rate and the neighboring radius decrease monotonically with epochs (one epoch being a full sequence of iterations through the dataset) (see the full algorithm in 4).
Figure 1: Mapping produced by a SOM with an input layer composed of 3 elements (RGB colors), and an inner layer composed of a grid of 50x50 elements. Left: the continuous mapping defined by the grid of prototypes (weights of inner layer units). Center: the initial dataset, composed of randomly chosen 3D points with values in [0,1] on each dimension (each point can be displayed as an RGB color). Right: the mapping is produced by finding a 2D manifold in the 3D space of the data that optimizes the description of all original points.

SOM allows to build a low dimensional mapping between the input space and the space of the inner layer (see Figure 1). In the described algorithm implementations (algorithms 2 and 1) a 1-Dimensional space has been chosen for the inner layer. Indeed the radial-basis function in 8 is based on a distance between two scalar indices. If for instance a 2-Dimensional description of the hidden space was chosen, the radial basis function would be based on an euclidean distance between two 2-dimensional points (the current prototype and the winner) in the space where the inner layer grid was laid out.

The low-dimensional mapping defined by a SOM is discretized, meaning that the activation of the inner layer can define only discrete points in the space of the mapping, defined by the position of the units in an imaginary grid that is laid out on that space. Nevertheless a multivariate interpolation can be applied (for instance a radial-basis interpolation) so that a pattern of activations in the inner layer gets related to a single point in the continuous space of the mapping (see Figure 2).

Input: \( q \): a point in the continuous space of the mapping

Data: \( u \in \mathbb{R}^K \): inner layer activations
\( W \in \mathbb{R}^{K \times M} \): weights
\( \hat{x} \in \mathbb{R}^M \): generated input pattern
\( \sigma \): smoothness

begin
for \( j \leftarrow 1 \) to \( K \) do
\( u_j \leftarrow \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{(j-q)^2}{2\sigma^2}} \)
\( \hat{x} \leftarrow W^T u \)
end

Algorithm 3: Radial basis interpolation.

Comparing the algorithms 2 and 4 we can see how they are strictly related. Indeed the SOM algorithm is a minimization of an energy function very similar to 3, where the \( \phi \) operator defined in 1 is substituted to the \( \phi \) operator defined in 8 and the weights \( w_j \) stand for the centroids \( c_j \). Incidentally the SOM learning algorithm can be also be described with batch mode (see algorithm 5).
Algorithm 4: SOM learning algorithm - online version

**Input:** \( \mathbf{X} \in \mathbb{R}^{N,M} \): the input dataset  
\( \mathbf{W} \in \mathbb{R}^{K,M} \): weights of the SOM (each row is a prototype)  
\( \eta_{\text{init}} \): initial learning rate  
\( \sigma_{\text{init}} \): initial neighboring radius  
\( \tau \): decay window  
\( T \): number of epochs

for \( t \leftarrow 0 \) to \( T - 1 \) do

\[ \eta \leftarrow \eta_{\text{init}} e^{-\frac{t}{\tau}} \]

\[ \sigma \leftarrow \sigma_{\text{init}} e^{-\frac{t}{\tau}} \]

shuffle \( \mathbf{X} \)

for \( i \leftarrow 1 \) to \( N \) do

\[ r_i = \arg \min_k ||\mathbf{x}_i - \mathbf{w}_k|| \]  
// Index of the winner.

for \( j \leftarrow 1 \) to \( K \) do

\[ \phi_{i,j} \leftarrow e^{-\frac{||j - r_i||^2}{2\sigma^2}} \]  
// Update operator.

\[ \mathbf{w}_j \leftarrow \mathbf{w}_j + \eta \phi_{i,j} (\mathbf{x}_i - \mathbf{w}_j) \]  
// Updating of weights.

Algorithm 5: SOM learning algorithm – batch version

**Input:** \( \mathbf{X} \in \mathbb{R}^{N,M} \): input dataset  
\( \mathbf{W} \in \mathbb{R}^{K,M} \): weights of the SOM (each row is a prototype)  
\( \sigma_{\text{init}} \): initial neighboring radius  
\( \tau \): decay window

\( t \leftarrow 0 \)

while \( \sum_{j=0}^{K} ||\Delta \mathbf{w}_j|| < \epsilon \) do

\[ \sigma \leftarrow \sigma_{\text{init}} e^{-\frac{t}{\tau}} \]

for \( i \leftarrow 1 \) to \( N \) do

\[ r_i = \arg \min_k ||\mathbf{x}_i - \mathbf{w}_k|| \]  
// Index of the winner.

for \( j \leftarrow 1 \) to \( K \) do

\[ \phi_{i,j} \leftarrow e^{-\frac{||j - r_i||^2}{2\sigma^2}} \]  
// Update operator.

for \( j \leftarrow 1 \) to \( K \) do

\[ \mathbf{w}_j \leftarrow \frac{\sum_{i=1}^{N} \phi_{i,j} \mathbf{x}_i}{\sum_{i=1}^{N} \phi_{i,j}} \]  
// Updating of clusters.

\( t \leftarrow t + 1 \)

4 Supervised Topological Maps

As we saw before, the implementation of the \( \phi \) WTA operator determines which algorithm between k-means clustering and SOM is used. These two implementations differ in the smoothness of WTA competition. While in k-means a simple step function divides the winner prototype from all the others, in SOMs a smooth function (typically a radial basis) based on the distance of prototypes from the winner determines the neighborhood of the to-be-updated prototypes. We will now define another kind of WTA operator depending on 1) the Euclidean distance between input patterns and the prototypes; 2) the Euclidean distance from prototypes and the winner prototype; 3) the Euclidean distance of prototypes...
from an extrinsically given point in the low-dimensional mapping space, for each input pattern:

\[ r_i = \arg \min_k ||x_i - w_k|| \]

\[ \phi_{i,j} = e^{-\frac{||j-r_i||^2}{2\sigma^2}} e^{-\frac{||j-t_i||^2}{2\sigma^2}} \]  

By means of the WTA operator in eq. 10 we can now tell the learning process where to put the internal representations for a category of data. The two parts of the WTA operator will take two different roles in the update process: 1) the radial basis of the distance between the prototypes and the winner will define the smoothing of prototypes while moving from a label to another in the mapping space; 2) the radial basis of the distance between the prototypes and the label points will define the center of attraction for prototypes of that category. When the update process is complete a low dimensional mapping emerges in the STM in which prototypes keep close to their labeling positions depending on their distance from the relative prototype (see Figure 3). Such a mapping can be used to generate new items starting from any randomly chosen point in the mapping space.

Figure 3: Example of mapping obtained by training an STM with 3 input units (RGB) and a 10x10 grid of inner units. On the 2-dimensional mapping on which the grid of color prototypes is laid out you can also see the three label points categorizing all data-points. Each RGB input pattern is assigned to one of the points depending on whether the red, green or blue channel has higher amplitude than the others.
Algorithm 6: STM learning algorithm – batch version

Input: \( X \in \mathbb{R}^{N,M} \): input dataset
\( \mathbf{W} \in \mathbb{R}^{K,M} \): weights of the STM (each row is a prototype)
\( \sigma_{r_{\text{init}}} \): initial neighboring radius
\( \sigma_{l_{\text{init}}} \): initial label radius
\( \tau \): decay window

\( t \leftarrow 0 \)

while \( \sum_{j=0}^{K} ||\Delta \mathbf{w}_j|| < \epsilon \) do

\[ \sigma_r \leftarrow \sigma_{r_{\text{init}}} e^{-\frac{t}{\tau}} \]
\[ \sigma_t \leftarrow \sigma_{l_{\text{init}}} e^{-\frac{t}{\tau}} \]

for \( i \leftarrow 1 \) to \( N \) do

\[ r_i = \arg \min_k ||x_i - \mathbf{w}_k|| \] // Index of the winner.

for \( j \leftarrow 1 \) to \( K \) do

\[ \phi_{i,j} = e^{-\frac{||j-r_i||^2}{2\sigma_r^2}} \]
\[ \phi_{i,j} = e^{-\frac{||j-t_i||^2}{2\sigma_t^2}} \] // Update operator.

for \( j \leftarrow 1 \) to \( K \) do

\[ \mathbf{w}_j \leftarrow \frac{\sum_{i=1}^{N} \phi_{i,j} x_i}{\sum_{i=1}^{N} \phi_{i,j}} \] // Updating of clusters.

\( t \leftarrow t + 1 \)

5 Using STMs

We give here two examples of the use of STMs for data generation.

First we show how to create a supervised mapping from the MIST dataset of standard handwritten digits (LeCun et al., 1998). The MNIST dataset is composed of 60,000 28x28 pixel images of the 10 digits (see Figure 4). An STM composed of a 28x28 input layer and a 10x10 inner layer was deployed. We defined the labeling points in the space of the inner layer as in Figure 5a. After learning the prototypes of the network were disposed according to the labeling, as it can be seen in Figure 5b where the weights of each prototype are plotted in their position in the grid of the inner layer units. Once the mapping was obtained we could produce new images through radial-basis interpolation (see Figure 2) from randomly chosen points in the continuous 2-dimensional space of the mapping. Figure 5c shows some samples of such generated images.

Another example was implemented using the Chicago Face Database (CFD – Ma et al., 2015). The CFD consists of 158 high-resolution, standardized photographs of Black and White males and females between the ages of 18 and 40 years. Each photograph is labeled based on eight categories: asian female; asian male; black female; black male; latino female; latino male; white female; white male. The original RGB 2444x1718 pixel photographs were further processed to obtain 152x107 8bit gray-scale images. A sample of the original photographs and their processed version is shown in Figure 6. An STM composed of a 152x107 input layer and a 10x10 inner layer was deployed. We defined the labeling points in the space of the inner layer as in Figure 7a. After learning the prototypes of the network were disposed according to the labeling, as it can be seen in Figure 7b where the weights of each prototype are plotted in their position in the grid of the inner layer units. Once the mapping was obtained we could produce new images through
Figure 5: Mapping produced with the STM algorithm on the MNIST dataset. a) The labeling points in the mapping space. Each pattern that is tagged with a digit label in the MNIST dataset gets a representation that is close to the corresponding point in the mapping. b) Weights of the STM after learning. The weights for each inner units are plotted in the corresponding position on the inner layer grid; c) images generated from interpolations of a random set points in the continuous space of the mapping.

radial-basis interpolation (see [2]) from randomly chosen points in the continuous 2-dimensional space of the mapping. Figure [8] shows some samples of such generated images.

Figure 6: A sample of photographs from the Chicago Face Database. Above, the original photographs from the dataset. Below, the processed versions of the CFD used in this paper.

6 Discussion

We showed here a variant of the algorithm used for Self Organizing Maps (SOMs) which allows to easily obtain a low dimensional mapping of the input space in a supervised manner, by constraining the positions of the representations in the mapping to keep themselves close to their corresponding labeling positions. The new family of algorithms, which we call Supervised Topological Maps (STMs), is defined by changing the winner-takes-all operator in SOMs so that it is also sensible to the distance between prototypes and labels in the internal space of the mapping. The finding that a general family of algorithms can be defined where the WTA operator identifies the differences between individual algorithms, have its origins in the strict relation between the k-means algorithm and SOMs. Indeed, as we showed the two algorithms share many features and the main difference is the way WTA competition is used. This idea was already implicitly present in the work of Kohonen, in particular in his description of the Learning Vector Quantization algorithm (LVQ – Kohonen). LVQ is a classification algorithm which adapts the position of the winner prototypes based on their
labeling. Following the notation used in this paper we can describe LVQ by defining its WTA operator as:

\[ r_i = \arg \min_k ||x_i - w_k|| \]

\[ \phi_{i,j}^{\text{dist}} = \begin{cases} 
1 & \text{if } j = r_i \\
0 & \text{otherwise}
\end{cases} \]

\[ \phi_{i,j}^{\text{lab}} = \begin{cases} 
1 & \text{if } j = t_i \\
-1 & \text{otherwise}
\end{cases} \]

\[ \phi_{i,j} = \phi_{i,j}^{\text{dist}} \phi_{i,j}^{\text{lab}} \tag{11} \]

where \( i \) is the index of the input pattern, \( t_i \) is the label prototype position position for the \( i^{th} \) input pattern and \( j \) is the position of the prototype currently taken into account. As in SOMs, although it is a classification algorithm, LVQ algorithm is strictly related to as k-mean clustering differing from it in the way the WTA operator is filtered by a function of the position of prototypes in the cluster space. As in STM its function of the internal position also depends on an extrinsic labeling of the cluster space.

We saw how adapting the low-dimensional mapping in a supervised way as in STMs allows for internal representations of data that are easy to interpret and to be used for generation of new data. A similar result is nowadays commonly achieved by using probabilistic generative models such as variational autoencoders (VAE – Kingma and Welling, 2013) or adversarial autoencoders (AAE – Makhzani et al., 2015). While these latter algorithms rely on parametric probability distributions for the shaping of the space of internal representations, the methods described here are a non-parametric deterministic way of modeling the space of internal representations. Probabilistic generative models are a better choice when a robust statistical definition of the population from which data comes out is required as well a formal level of reliability that new generated samples come from the same population of given data. On the other side non-parametric methods as the ones described here seem to be an easier way to model the internal representations of neural networks for practical issues. Moreover, the local update methods described here could shed a new light on the possible ways in which neural mappings from different sensory or motor modalities are synchronized together in the central nervous systems of animals.

Another difference from the commonly used neural network algorithms consists in the fact that STMs as described here are shallow networks and the prototypes cannot be deeply non-linear functions of the inputs. Nevertheless it could be shown that a STM layer can substitute the internal layer of a deep neural network with few changes. It was not the focus of this paper to show such a possibility. The demonstration of how to use STMs as deep layers a neural network (e.g. a deep autoencoder) will be the aim of a future work.

Concluding, a new family of algorithms, namely STMs, was described which allows for the supervised determination of the internal representations in a neural mapping.

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Figure 7: Mapping produced with the STM algorithm on the CFD dataset. a) The labeling points in the mapping space. Each pattern that is tagged with a digit label in the MNIST dataset gets a representation that is close to the corresponding point in the mapping. Labelings are: AF: asian female; AM: asian male; BF: black female; BM: black male; LF: latino female; LM: latino male; WF: white female; WM: white male. b) Weights of the STM after learning. The weights for each inner units are plotted in the corresponding position on the inner layer grid.
Figure 8: Generation of Images form the CFD mapping. Patterns are generated from interpolations of a random set points in the continuous space of the mapping.