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Self-Organizing Maps for Exploration of Partially Observed Data and Imputation of Missing Values

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Abstract

The self-organizing map is an unsupervised neural network which is widely used for data visualisation and clustering in the field of chemometrics. The classical Kohonen algorithm that computes self-organizing maps is suitable only for complete data without any missing values. However, in many applications, partially observed data are the norm. In this paper, we propose an extension of self-organizing maps to incomplete data via a new criterion that also defines estimators of the missing values. In addition, an adaptation of the Kohonen algorithm, named missSOM, is provided to compute these self-organizing maps and impute missing values. An efficient implementation is provided. Numerical experiments on simulated data and a chemical dataset illustrate the short computing time of missSOM and assess its performance regarding various criteria and in comparison to the state of the art.

Keywords: Self-organizing maps, partially observed data, missing data imputation, robustness to missingness mechanism

1. Introduction

In chemometrics, data exploration is essential and is generally the first part of the analysis of any dataset. With the explosion of data volume in many fields of application due to big data, the structure of data is often hidden behind the massive data and difficult to detect. This increases the importance of data exploration methods providing meaningful information on the internal structure and correctness of the data, as well as the relationships and redundancies among the variables. The

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initial understanding of the data gained by exploratory data analysis is particularly useful for data modeling.

Common tasks of data exploration are visualization and clustering of the data. While there is plethora of methods addressing one of the tasks, self-organizing maps simultaneously provide both a low-dimensional visual data representation in form of a map and a clustering of the observations. Introduced by [1], this approach consists in mapping the data and performing vector quantization of the input space while preserving topological properties of the data. Self-organizing maps have become very popular in many applications, since they provide easily interpretable results with a global view of the data. Among others, self-organizing maps are widely used in chemometrics [2, 3, 4, 5, 6, 7], but also in biology [8], humanities [9], industry, such as health monitoring of aircraft engines [10]. Many variants of the standard self-organizing map have been developed, such as Generative Topographic Mapping [11], which is a probabilistic version of the self-organizing map, or extensions to more complex data types (mixed, textual, etc.) [12, 13] demonstrating the relevance of self-organizing maps until today.

A common issue with datasets in most fields of application are missing data. Data may be incomplete for a large variety of reasons. In surveys, for instance, they occur due to non-responses questions that affect privacy [14, 15, 16]. In industrial applications and chemometrics, measuring instruments may have malfunctions or detection limits yielding erroneous and missing entries [17, 18]. In medical research, missing data can occur in clinical trials when patients abandon or stop taking the treatment for a certain period of time [19, 20, 21]. Missing data also frequently occur in chemical [22, 23] and environmental [24] studies. Moreover, concerning huge databases, merging several datasets from different sources can also result in missing data, as some entries may not be recorded at all for some of the sources.

The impact of missing data on statistical results can be serious, leading to biased estimates, loss of information, decreased statistical power, increased standard errors, and weakened generalizability of findings. However, for a long time, in statistics, missing data have been treated in a very simple and inappropriate way, either by deletion of incomplete measurements or by basic data completion by mean or median values. This has changed during the last decades, by the development of many statistical methods that account for missing data in a meaningful way. There are two general approaches to deal with missing data: either a statistical method is directly adapted to the partially observed data, or first an appropriate imputation method is applied to complete the data such that

the statistical method of interest can be used on the completed or augmented data.

In this paper we are interested in self-organizing maps in the presence of missing data. This problem has been considered among others by [25] by simply restricting all vector calculations to the observed entries. As such, all observed data entries are taken into account in the algorithm. However, the method performs rather poorly when the number of incomplete observations with multiple missing entries is large. Moreover, the imputation of missing data is done afterwards by replacing missing entries by the closest features on the learned map. Similar approaches are presented in [26, 27, 28, 29, 30].

We have the ambition to combine the tasks of imputation and learning the map by a principled approach. Our motivation is the fact that any non trivial imputation method is based on some data model, and so it is natural to use the self-organizing map for imputation. Conversely, a better map may be learned when data are complete. Thus, treating both tasks simultaneously may be beneficial for the two of them.

Our approach can be viewed as an extension of the standard Kohonen algorithm for self-organizing maps and the principle of our method is given in Section 2. A mathematical presentation of the method, a new loss function that encodes our double goal of imputation and learning a self-organizing map and two algorithmic solutions are given in Section 3. Moreover, Section 4 provides an extensive numerical study assessing the robust performance of our method in various settings and in comparison to alternative methods from the literature.

2. The new method in a nutshell

This section presents the principle of our new method for self-organizing maps for partially observed data. To start with, we recall the classical self-organizing map. Let x_1, \dots, x_n be n observations or measurements of dimension p . A self-organizing map represents a nonlinear projection of the high-dimensional data onto a low-dimensional subspace. This subspace is a two-dimensional map represented as a regular grid composed of K fixed neurons. This fixed spatial arrangement of the neurons on the map is the key for the preservation of the topology of the input data when projected onto the map. Every neuron k is associated with a p -dimensional prototype vector w_k , also called code vector, that is to be learned. The prototype vectors define a discretization of the data space, and each observation x_i is assigned to its closest prototype. Ideally, prototype vectors

of neighboring neurons on the grid are close one to another, so that data points x_i that are close in the input space are also close on the map.

The Kohonen algorithm computes the self-organizing map for complete data in an iterative fashion. One randomly picked observation x_i is treated at each iteration. First, the winning neuron or best matching unit is determined, which is the neuron whose prototype is the closest to measurement x_i . Then, all code vectors w_k are updated by attracting them towards the measurement x_i . The attraction is the strongest for the winning neuron and very weak for the neurons that are far from the winning neuron. Those updates eventually result in an ordered map, where neighboring neurons have similar prototype vectors.

Now, when some of the measurement vectors x_i contain missing entries, the Kohonen algorithm is not applicable anymore. We propose to learn the missing entries while learning the map in the following way. Our algorithm is the following: starting from some initial imputed values, like the mean values computed over the observed entries, select every measurement x_i once, determine its winning neuron by considering the distance only over the observed entries of x_i and then update the code vectors just as in the classical Kohonen algorithm. Then, perform an update of the imputed values using a weighted means of the closest code vectors of the partially observed measurement. Repeat this procedure until convergence. A full description is provided in Algorithm 3.

This algorithm performs both data visualization and imputation of the incomplete data. Interestingly, it is as fast as the standard Kohonen algorithm, since the update of the imputed values is immediate.

3. Self-organizing maps with incomplete data

In this section we first formally state the classical self-organizing map, before introducing the new loss function and two algorithms for the computation of self-organizing maps with partially observed data and missing data imputation.

3.1. Classical Kohonen algorithm

The data matrix containing the measurements is denoted by $X = [x_1, \dots, x_n] \in \mathbb{R}^{n \times p}$. The arrangement of the neurons on the map is given by some neighborhood function $V_\lambda : \{1, \dots, K\}^2 \mapsto \mathbb{R}_+$. The neighborhood radius $\lambda > 0$ describes the zone of influence around a neuron. The best

Algorithm 1: Standard Kohonen algorithm

Input: Data matrix X , size and topology of the map, neighborhood function V_λ , sequence of radii $(\lambda_t)_{0 \leq t \leq T}$ and learning steps $(\varepsilon_t)_{0 \leq t \leq T}$.

Initialize code vectors $W^{(0)}$;

Initialize the counter of iterations: $t = 0$;

while *not converged* **do**

 Increment t : Set $t = t + 1$;

 Choose an observation $i \in \{1, \dots, n\}$ randomly ;

 Assignment: Compute winning neuron $\ell = h(x_i, W^{(t-1)})$;

 Update code vectors:

for $k = 1, \dots, K$ **do**

$w_k^{(t)} = w_k^{(t-1)} + \varepsilon_t V_{\lambda_t}(k, \ell) (x_i - w_k^{(t-1)})$.

end

end

Output: Code vectors $W^{(t)}$.

prototype vectors of the self-organizing map are defined as the minimum of the loss function F defined by

$$F(W) = \frac{1}{2n} \sum_{i=1}^n \sum_{k=1}^K V_\lambda(k, h(x_i, W)) \|x_i - w_k\|_2^2, \quad (1)$$

where $W = [w_1, \dots, w_K] \in \mathbb{R}^{p \times K}$ is the matrix of K prototype vectors and $h : \mathbb{R}^p \times \mathbb{R}^{p \times K} \mapsto \{1, \dots, K\}$ denotes the allocation function, attributing the closest prototype to a data point x w.r.t. the Euclidean distance, defined as

$$h(x, W) = \arg \min_{1 \leq k \leq K} \|x - w_k\|_2. \quad (2)$$

The loss F takes into account all distances between every measurement and all code vectors, weighted by the neighborhood function evaluated on the corresponding neurons. As a result, code vectors that minimize the loss are similar if they are close on the map. In the specific case where the neighborhood function satisfies $V_\lambda(k, \ell) = 0$ for all $k \neq \ell$, the loss F is the criterion minimized by the k -means algorithm.

To compute the minimum of loss F , [31] showed that in the given framework a gradient descent algorithm can be used, referred to as the Kohonen stochastic algorithm. For a randomly picked

observation x_i with winning neuron $\ell = h(x_i, W^{(t)})$, the updates of the code vectors are given by

$$w_k^{(t+1)} = w_k^{(t)} + \varepsilon_t V_\lambda(k, \ell)(x_i - w_k^{(t)}), \quad (3)$$

where $(\varepsilon_t)_{t \geq 0}$ is a sequence of decreasing learning steps. This update attracts all prototypes towards observation x_i . It is also common to shrink the neighborhood by using a decreasing sequence of radii $(\lambda_t)_{t \geq 0}$ in the neighborhood function V_λ . The algorithm is summarized in Algorithm 1.

3.2. Notation for incomplete data

Now we consider an incomplete $n \times p$ data matrix containing missing values. Let the matrix $M = (m_{i,j})_{i,j} \in \{0, 1\}^{n \times p}$ be the missing-data pattern which indicates where the entries are missing or masked, and that is defined by

$$m_{i,j} = \begin{cases} 1 & \text{if } x_{i,j} \text{ is observed} \\ 0 & \text{if } x_{i,j} \text{ is missing} \end{cases}$$

We denote X^{obs} the set of observed data values and X^{miss} the set of non-observed data entries hidden by the missing-data pattern M . The complete data are denoted by $X^{\text{compl}} = (X^{\text{obs}}, X^{\text{miss}})$. Likewise, for the observation vector x_i we denote by x_i^{obs} and x_i^{miss} the observed and unobserved entries, respectively, and, with some abuse of notation, $x_i^{\text{compl}} = (x_i^{\text{obs}}, x_i^{\text{miss}})$ is the complete vector, which also corresponds to the i -th row of X^{compl} .

Our goal is to adapt the model of self-organizing maps to partially observed data, and moreover, learn the values of the missing data. The motivation to treat these tasks simultaneously is that learning missing values requires a data model, and as we are interested in self-organizing maps it is natural to use this model for data imputation. At the same time, learning a map with completed data may give better results compared to using only the observed part X^{obs} of the data.

3.3. New loss function

We introduce a new loss function that considers both problems : finding the best self-organizing map and the best values for imputation of the missing data. In other words, by minimizing the new loss function F_{missom} we search for both the best code vectors $W \in \mathbb{R}^{p \times K}$ for the map and the best values for the missing data denoted by X^* chosen in the set of all possible values for the missing entries $\mathcal{X}^{\text{miss}}$.

To define the new criterion, an adaptation of the definition of the winning neuron is in order. In the presence of missing values, it is natural to restrict the Euclidean distance in (2) only to the observed entries. More precisely, for any vectors $x^{\text{obs}} \in \mathbb{R}^{p'}$ ($p' \leq p$), $m \in \{0, 1\}^p$ with $\sum_{j=1}^p m_j = p'$ and code vectors $W \in \mathbb{R}^{p \times K}$, we set

$$h^{\text{miss}}(x^{\text{obs}}, m, W) = \arg \min_{1 \leq k \leq K} \|x^{\text{obs}} - w_k \odot m\|_2,$$

where $w_k \odot m$ denotes the p' -vector made of the elements $w_{k,j}$ of w_k such that $m_j = 1$. Now, we define the new loss as

$$F_{\text{missom}}(W, X^*) = \frac{1}{2n} \sum_{i=1}^n \sum_{k=1}^K V_\lambda(k, h^{\text{miss}}(x_i^{\text{obs}}, m_i, W)) \|(x_i^{\text{obs}}, x_i^*) - w_k\|_2^2,$$

where $m_i \in \mathbb{R}^p$ is the i -th row of the matrix M and $(x_i^{\text{obs}}, x_i^*)$ denotes the i -th measurement vector completed with x_i^* . Since

$$\|(x_i^{\text{obs}}, x_i^*) - w_k\|_2^2 = \|x_i^{\text{obs}} - w_k \odot m_i\|_2^2 + \|x_i^* - w_k \odot (\mathbf{1}_p - m_i)\|_2^2,$$

where $\mathbf{1}_p = (1, \dots, 1)^T \in \mathbb{R}^p$, the criterion F_{missom} can be decomposed into two parts according to the observed and the missing entries as

$$F_{\text{missom}}(W, X^*) = F_{\text{obs}}(W) + F_{\text{miss}}(W, X^*),$$

where $F_{\text{obs}}(W)$ is the part of the loss over the observed entries given by

$$F_{\text{obs}}(W) = \frac{1}{2n} \sum_{i=1}^n \sum_{k=1}^K V_\lambda(k, h^{\text{miss}}(x_i^{\text{obs}}, m_i, W)) \|x_i^{\text{obs}} - w_k \odot m_i\|_2^2,$$

and $F_{\text{miss}}(W, X^*)$ is the contribution of the imputed values X^* to the loss, defined as

$$F_{\text{miss}}(W, X^*) = \frac{1}{2n} \sum_{i=1}^n \sum_{k=1}^K V_\lambda(k, h^{\text{miss}}(x_i^{\text{obs}}, m_i, W)) \|x_i^* - w_k \odot (\mathbf{1}_p - m_i)\|_2^2.$$

Note that in the complete-data case, where the missing-data pattern is $M = \mathbf{1}_{n \times p}$, $F_{\text{miss}}(W, X^*) = 0$ for any W and any X^* , so that the criterion F_{missom} is equal to the one of the classical self-organizing map, that is, $F_{\text{missom}}(W, X^*) = F(W)$.

Algorithm 2: missSOM algorithm

Input: Incomplete data X^{obs} , missing-data pattern M , size and topology of the map, neighborhood function V_λ , sequence of radii $(\lambda_t)_{0 \leq t \leq T}$ and learning steps $(\varepsilon_t)_{0 \leq t \leq T}$.

Initialize imputed values $X^{*(0)}$ and code vectors $W^{(0)}$;

Initialize the counter of iterations: $s = 0$;

while *not converged* **do**

 Increment s : Set $s = s + 1$;

 Update code vectors by Kohonen Algorithm 1 on the augmented data with winning neurons obtained by h^{miss} instead of h :

$W^{(s)} \leftarrow \text{Kohonen}(X^{\text{aug}} = (X^{\text{obs}}, X^{*(s-1)}))$;

 Update imputed values: for i, j such that $m_{i,j} = 0$,

$$x_{i,j}^{*(s)} = \frac{\sum_{k=1}^K V_{\lambda_T}(k, h^{\text{miss}}(x_i^{\text{obs}}, m_i, W^{(s)})) w_{k,j}^{(s)}}{\sum_{k=1}^K V_{\lambda_T}(k, h^{\text{miss}}(x_i^{\text{obs}}, m_i, W^{(s)}))}.$$

end

Output: Code vectors $W^{(s)}$ and imputed data $X^{*(s)}$.

3.4. Minimization algorithm

For the minimization of $(W, X^*) \mapsto F_{\text{miss}}(W, X^*)$ on $\mathbb{R}^{K \times p} \times \mathcal{X}^{\text{miss}}$ we propose to alternate the minimization in W and X^* while keeping the other argument fixed.

For fixed X^* , the function $W \mapsto F_{\text{missom}}(W, X^*)$ is similar to the objective function F in (1) in the complete-data case applied to the augmented data $X^{\text{aug}} = (X^{\text{obs}}, X^*)$. The only difference lies in the definition of the winning neurons by h^{miss} that appear in the neighbourhood function V_λ . Thus, a Kohonen algorithm applied to X^{aug} can be used to find the best code vectors W .

In turn, when W is fixed, the minimization of $X^* \mapsto F_{\text{missom}}(W, X^*)$ boils down to minimize $X^* \mapsto F_{\text{miss}}(W, X^*)$. This problem has a unique explicit solution given for all $1 \leq i \leq n$ and j such that $m_{i,j} = 0$ by

$$x_{i,j}^* = \frac{\sum_{k=1}^K V_\lambda(k, h^{\text{miss}}(x_i^{\text{obs}}, m_i, W)) w_{k,j}}{\sum_{k=1}^K V_\lambda(k, h^{\text{miss}}(x_i^{\text{obs}}, m_i, W))}. \quad (4)$$

That is, the imputed values are a weighted mean of the prototype vectors weighted according to the neighborhood function.

To summarize, the algorithm updates imputed values for the missing data and applies the classical Kohonen algorithm with adjusted winning neuron function h^{miss} to learn the map. This is repeated until convergence or until a maximum number of iterations chosen by the user is attained. The algorithm is described in Algorithm 2.

As initial values for the imputed values X^* , one can simply impute the sample mean or median of the variables obtained over the observed entries.

3.5. Accelerated version

Algorithm 2 happens to be expensive in terms of computing time, in particular when the number of iterations is large, since the entire standard Kohonen algorithm is carried out during each iteration. A speed up is obtained by intertwining updates of the missing data and the iterations of the Kohonen Algorithm 1. More precisely, we propose to update the missing data at every epoch, that is, after every pass through the data. This procedure gives rise to Algorithm 3. As such, the Kohonen algorithm is carried out only once, while in the initial Algorithm 2, the entire Kohonen algorithm is applied repeatedly. Thus the computing time of the accelerated version of missSOM is comparable to the computing time of the standard Kohonen Algorithm 1, since the update of the imputed values is fast.

While the first version of the missSOM algorithm has some theoretical justification, the accelerated version lacks this foundation. A numerical study given in Appendix 6.1 shows that the Algorithms 2 and 3 provide very similar maps and hence justifies the utilization of the accelerated version, which achieves a significant gain in computing time.

Note that while the selection of the observations x_i in Algorithm 3 is deterministic, it is possible to use a random selection scheme.

4. Numerical experiments

In this section, the performance of the missSOM method is evaluated and compared to alternative methods in various settings.

4.1. Performance criteria

Performance is assessed in terms of topographic and quantization properties of the map, the quality of imputed values, clustering properties and computing time. Now denote W^* the code

vectors of the final self-organizing map, X^* the imputed values and $\hat{x}_i = (x_i^{\text{obs}}, x_i^*)$ the completed observation vectors.

The quality of the map can be evaluated by two criteria. First, the *quantization error* defined as the average of the squared distance between the observations and their nearest prototype vector given by

$$E = \frac{1}{n} \sum_{i=1}^n \|\hat{x}_i - w_{h(\hat{x}_i, W^*)}\|_2^2,$$

informs on whether the prototype vectors are good representations of the data. Second, the *topographic error* evaluates the preservation of the topology of the data by the proportion of observations for which the winning neuron and the second closest neuron are not neighbors, i.e. not connected on the grid. It is defined as

$$T = \frac{1}{n} \sum_{i=1}^n e(\hat{x}_i),$$

where

$$e(\hat{x}_i) = \begin{cases} 0 & \text{if the neurons } h(\hat{x}_i, W^*) \text{ and } v(\hat{x}_i, W^*) \text{ are adjacent} \\ 1 & \text{otherwise} \end{cases}$$

with $v(\hat{x}_i, W^*) = \arg \min_{j \neq h(\hat{x}_i, W^*)} \|\hat{x}_i - w_j^*\|_2^2$ the second closest neuron to measurement \hat{x}_i . The topographic error is small if the map is well organized and ordered.

Self-organizing maps define a clustering of the data, where each prototype vector represents one cluster. When the map is well ordered, neighboring neurons can be grouped together to form larger clusters and so a clustering into a small number of groups can be derived. In our study we use hierarchical ascending classification (HAC) based on Ward’s criterion [32] to obtain the clusterings into three or four groups. The quality of the clustering is evaluated by the *adjusted Rand index* (ARI) [33], measuring the similarity of two partitions.

Finally, we consider the *imputation error* defined as the root mean square error to quantify the quality of the imputed values compared to the true missing values.

4.2. Datasets

For the numerical experiments, we consider two settings. For the first, the dataset *wine* from the UCI machine learning repository [34] is used, which contains the results of a chemical analysis of 178 wines on 13 quantitative variables. A categorical variable with three classes representing the type of wine will be used to evaluate the performance in terms of clustering into three groups. We

generate 20 perturbed datasets by adding gaussian noise with mean 0 and standard deviation equal to one tenth of the mean value in each variable.

For the second setting, we simulate 20 datasets from a multivariate gaussian mixture with dimension $p = 5$, four equal-sized groups and $n = 2000$ observations. For every dataset, the 4 gaussian means are drawn independently from a centered normal distribution with standard deviation equal to 10.

In both settings, we generate missing values using the `ampute` function from the R package `mice` [35]. Different proportions of missing values, namely 5%, 20% and 40%, and different mechanisms of missingness are considered. The literature on missing data traditionally distinguishes the three mechanisms that lead to missingness [36]. The mechanism is said to be *missing completely at random* (MCAR), when the causes of missing values are independent from the data and the probability of being absent is the same for all items. When the probability that a value is missing depends only on the values of the observed variables, the mechanism is called *missing at random* (MAR). Finally, when the probability of being absent also depends on the unobserved value, the mechanism is called *missing not at random* (MNAR).

4.3. Alternative methods

We compare *missSOM* to the state of the art. The simplest method (referred to as *deletion* in the tables) consists in deleting the observations containing missing values and applying the standard Kohonen algorithm to the remaining data. Incomplete observations are classified after the map is built by assigning them to their closest prototypes for distance restricted only to the observed entries and missing entries are imputed by the values of the prototypes. Another very basic approach (here called *mean*) is the imputation by the mean of the observed variables and applying the standard Kohonen algorithm to the augmented data.

Cottrell is a method for self-organizing maps dealing directly with missing data [25] by adapting the Kohonen algorithm by simply restricting all vector calculations to the observed entries. To use this map for data imputation, the values of the closest prototypes of the incomplete observations are used. This method is the approach that is the closest to the *missSOM* algorithm.

The literature provides numerous general imputation methods that are not specifically related to self-organizing maps. In our study, we consider a non-parametric model using random forests (*missForest*) provided by the `missForest` package [37, 38] which consists in predicting the missing

values using a random forest trained on the observed parts of the dataset. Moreover, we consider imputation by a k -nearest neighbors approach [39] (*knn*) implemented in the VIM package [40]. Here, missing values are imputed iteratively by the weighted average of their k closest observations. Finally, assuming that data come from a gaussian mixture, the *Amelia* package [41] performs imputation using the expectation-maximization algorithm and a bootstrap approach to iteratively estimate missing values. In the following numerical experiments, the imputation methods are used to create complete datasets, to which the classical Kohonen algorithm is applied.

In addition, [42] developed an extension of the k -means algorithm for incomplete data (*kpod*). It consists in alternating the imputation of the missing data by the centroids of the clusters and performing an iteration of k -means on the completed data. This approach is similar in spirit to the accelerated version of the *missSOM* algorithm and we compare *missSOM* to *kpod* in terms of clustering.

4.4. Parameters of the methods

The *missSOM* algorithm is applied with the default parameters in the package *missSOM*. That is, the map has a hexagonal topology and is a grid composed of $K = 8 \times 6$ neurons. The neighborhood function is a gaussian and the sequence $(\lambda_t)_{t \leq T}$ decreases from $\lambda_0 = 4.36$ to $\lambda_T = 0.5$. The maximum number of epochs is $T = 100$.

For the alternative methods, the maximum number of iterations is set to 100 and for the other parameters the default values are used.

4.5. Comparison to the state of the art

Table 1 and 2 present the results for the comparison of *missSOM* to the state of the art on the wines data and for a multivariate gaussian mixture, respectively.

Our *missSOM* algorithm achieves excellent results in terms of the topographic error, especially when the amount of missing data is elevated, regardless of the missingness mechanism. This means that the map is very well ordered.

As an imputation method, *missForest* is unbeaten regardless of the missingness mechanism and the percentage of missing data. However, *missSOM* performs very well, mostly being among the best methods. However, *missForest* provides self-organizing map of poorer quality and is quite costly in terms of computing time.

The *deletion* method is pointless as it does not work when there are too many missing values. When results are obtained, its quantization and imputation errors are among the worst of all methods on the wines data, while it performs better on gaussian mixture data. The *deletion* method with at least 20% missing data cannot be applied to a small dataset like wines data as the number of complete observations remaining is smaller than the size of the map.

The *kpod* method has an excellent ARI on the wines data except when 40% of data are missing with a missingness mechanism MAR or MNAR. But unlike *missSOM* it does not provide any map and is quite costly in terms of computing time.

Cottrell's method is the most similar method to *missSOM*. We observe that *missSOM* has the better topographic error, while *Cottrell* achieves slightly lower quantization errors. The latter has been expected, as this is a consequence of the imputation by the closest prototype vector, which is optimal in terms of the quantization error. Concerning the imputation method, *missSOM* outperforms *Cottrell* on the wine data, while *Cottrell* is doing better for small proportions of missing data on the gaussian data, but again *missSOM* is the better imputation method when 40% of the data are missing. This comforts the use of *missSOM* with respect to *Cottrell*, especially in the case where not only a self-organizing map is desired, but also good imputation.

5. Conclusion

In this paper, we have proposed an extension of the self-organizing map for partially observed data, referred to as *missSOM*. The proposed method addresses simultaneously the two problems of computing a self-organizing map and imputing missing values. A numerical study assesses the good performance of *missSOM* regarding various criteria and in comparison to the state of the art. While this paper focuses on the standard Kohonen algorithm, the next step now is to transfer the approach to the existing modern variants of self-organizing maps to enable them to deal with missing data.

6. Appendix

6.1. Validation of accelerated missSOM algorithm

Table 3 compares the results of the basic missSOM Algorithm 2 and its accelerated version Algorithm 3 on the simulated gaussian mixture data in various conditions. On the one hand, for all settings the errors are totally equivalent. This indicates that the accelerated version provides the same self-organizing maps and very similar imputations as the basic missSOM algorithm. On the other hand, we see that in terms of computing time we gain two orders of magnitude. Hence, the use of the accelerated algorithm instead of the basic version is completely justified.

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Algorithm 3: Accelerated missSOM algorithm

Input: Incomplete data matrix X^{obs} , missing-data pattern M , size and topology of the map, neighborhood function V_λ , sequence of radii $(\lambda_t)_{0 \leq t \leq T}$ and learning steps $(\varepsilon_t)_{0 \leq t \leq T}$.

Initialize imputed values $X^{*(0)}$ and code vectors $W^{(0)}$;

Initialize the number of epochs: $t = 0$;

while *not converged* **do**

 Increment t : Set $t = t + 1$;

 Set $\tilde{W}^{(0)} = W^{(t-1)}$;

for $i = 1, \dots, n$ **do**

 Assignment: Compute winning neuron $\ell = h^{\text{miss}}(x_i^{\text{obs}}, m_i, \tilde{W}^{(i-1)})$;

 Update code vectors:

for $k = 1, \dots, K$ **do**

$$\quad \quad \quad \left| \quad w_k^{(i)} = \tilde{w}_k^{(i-1)} + \varepsilon_t V_{\lambda_t}(k, \ell) \left((x_i^{\text{obs}}, x_i^{*(t-1)}) - \tilde{w}_k^{(i-1)} \right) . \right.$$

end

end

 Set $W^{(t)} = \tilde{W}^{(n)}$;

 Update imputed values: for i, j such that $m_{i,j} = 0$,

$$x_{i,j}^{*(t)} = \frac{\sum_{k=1}^K V_{\lambda_t}(k, h^{\text{miss}}(x_i^{\text{obs}}, m_i, W^{(t)})) w_{k,j}^{(t)}}{\sum_{k=1}^K V_{\lambda_t}(k, h^{\text{miss}}(x_i^{\text{obs}}, m_i, W^{(t)}))} .$$

end

Output: Code vectors $W^{(t)}$ and imputed data $X^{*(t)}$.

	5%			20%			40%		
	MCAR	MAR	MNAR	MCAR	MAR	MNAR	MCAR	MAR	MNAR
Topographic error									
missSOM	0.308 (0.040)	0.319 (0.043)	0.327 (0.049)	0.293 (0.052)	0.305 (0.058)	0.308 (0.039)	0.279 (0.047)	0.283 (0.044)	0.290 (0.052)
Cottrell	0.304 (0.045)	0.325 (0.042)	0.329 (0.041)	0.292 (0.039)	0.317 (0.057)	0.300 (0.047)	0.289 (0.031)	0.288 (0.060)	0.310 (0.055)
knn	0.327 (0.040)	0.314 (0.039)	0.345 (0.030)	0.314 (0.031)	0.315 (0.057)	0.320 (0.040)	0.321 (0.046)	0.321 (0.042)	0.321 (0.059)
missForest	0.309 (0.036)	0.318 (0.048)	0.324 (0.061)	0.331 (0.055)	0.320 (0.045)	0.332 (0.049)	0.293 (0.033)	0.322 (0.053)	0.301 (0.041)
mean	0.324 (0.052)	0.328 (0.038)	0.344 (0.049)	0.328 (0.038)	0.345 (0.037)	0.327 (0.043)	0.326 (0.028)	0.333 (0.041)	0.333 (0.057)
deletion	0.336 (0.046)	0.325 (0.038)	0.308 (0.060)	—	—	—	—	—	—
Quantization error									
missSOM	4.461 (0.545)	4.523 (0.687)	4.475 (0.693)	3.531 (0.549)	3.717 (0.673)	3.750 (0.546)	2.443 (0.438)	2.751 (0.310)	2.709 (0.395)
Cottrell	4.501 (0.595)	4.666 (0.706)	4.483 (0.633)	3.350 (0.478)	3.451 (0.476)	3.615 (0.542)	2.098 (0.333)	2.299 (0.294)	2.263 (0.280)
knn	4.428 (0.712)	4.683 (0.755)	4.726 (0.661)	3.986 (0.407)	4.198 (0.526)	4.120 (0.581)	3.428 (0.366)	3.295 (0.421)	3.449 (0.594)
missForest	4.273 (0.572)	4.734 (0.605)	4.646 (0.793)	3.748 (0.577)	4.046 (0.497)	4.122 (0.475)	2.904 (0.338)	3.177 (0.371)	2.957 (0.360)
mean	4.583 (0.58)	4.601 (0.677)	4.732 (0.732)	4.092 (0.513)	4.423 (0.671)	4.320 (0.570)	3.388 (0.510)	3.744 (0.475)	3.418 (0.473)
deletion	5.222 (0.067)	7.067 (1.155)	7.172 (1.064)	—	—	—	—	—	—
Imputation error									
missSOM	0.845 (0.060)	0.840 (0.098)	0.863 (0.083)	0.844 (0.028)	0.870 (0.038)	0.904 (0.035)	0.882 (0.022)	0.941 (0.029)	0.957 (0.025)
Cottrell	0.847 (0.061)	0.841 (0.087)	0.876 (0.092)	0.879 (0.038)	0.903 (0.040)	0.929 (0.047)	0.929 (0.020)	0.978 (0.031)	0.994 (0.028)
Amelia	0.887 (0.049)	0.894 (0.087)	0.922 (0.083)	0.902 (0.035)	0.922 (0.038)	0.947 (0.042)	1.006 (0.037)	0.998 (0.029)	1.034 (0.043)
knn	0.888 (0.049)	0.858 (0.107)	0.890 (0.083)	0.935 (0.030)	0.910 (0.021)	0.928 (0.033)	1.012 (0.028)	0.969 (0.022)	0.989 (0.030)
missForest	0.790 (0.051)	0.782 (0.078)	0.808 (0.083)	0.801 (0.031)	0.811 (0.020)	0.841 (0.038)	0.853 (0.020)	0.877 (0.025)	0.892 (0.026)
mean	1.018 (0.056)	1.022 (0.074)	1.053 (0.073)	0.994 (0.027)	1.028 (0.021)	1.065 (0.029)	1.002 (0.020)	1.037 (0.016)	1.066 (0.017)
deletion	0.875 (0.050)	0.879 (0.078)	0.927 (0.077)	—	—	—	—	—	—
ARI									
missSOM	0.646 (0.079)	0.605 (0.077)	0.615 (0.082)	0.603 (0.087)	0.540 (0.083)	0.531 (0.058)	0.502 (0.078)	0.414 (0.094)	0.407 (0.061)
Cottrell	0.619 (0.085)	0.608 (0.088)	0.616 (0.099)	0.563 (0.089)	0.557 (0.078)	0.533 (0.091)	0.505 (0.066)	0.430 (0.081)	0.446 (0.073)
kpod	0.747 (0.046)	0.735 (0.048)	0.742 (0.047)	0.683 (0.059)	0.667 (0.033)	0.674 (0.042)	0.578 (0.051)	0.489 (0.099)	0.483 (0.094)
knn	0.628 (0.118)	0.623 (0.111)	0.653 (0.098)	0.648 (0.077)	0.584 (0.078)	0.617 (0.094)	0.494 (0.067)	0.473 (0.083)	0.545 (0.066)
missForest	0.670 (0.106)	0.637 (0.074)	0.615 (0.081)	0.594 (0.094)	0.600 (0.086)	0.585 (0.072)	0.531 (0.104)	0.545 (0.075)	0.516 (0.079)
mean	0.605 (0.109)	0.587 (0.089)	0.606 (0.096)	0.548 (0.080)	0.533 (0.056)	0.534 (0.065)	0.449 (0.096)	0.356 (0.078)	0.396 (0.080)
deletion	0.632 (0.106)	0.584 (0.077)	0.596 (0.135)	—	—	—	—	—	—
Computational time									
missSOM	0.069 (0.003)	0.069 (0.002)	0.068 (0.002)	0.119 (0.006)	0.117 (0.004)	0.120 (0.004)	0.180 (0.011)	0.179 (0.011)	0.181 (0.012)
Cottrell	0.059 (0.002)	0.060 (0.002)	0.058 (0.002)	0.098 (0.070)	0.096 (0.067)	0.098 (0.070)	0.115 (0.082)	0.114 (0.088)	0.107 (0.069)
Amelia	0.058 (0.006)	0.061 (0.007)	0.060 (0.008)	0.160 (0.027)	0.143 (0.042)	0.138 (0.019)	1.451 (0.293)	0.834 (0.411)	0.819 (0.276)
kpod	0.174 (0.080)	0.180 (0.067)	0.218 (0.062)	0.177 (0.070)	0.217 (0.121)	0.250 (0.118)	0.149 (0.035)	0.218 (0.102)	0.150 (0.048)
Knn	0.184 (0.072)	0.198 (0.102)	0.182 (0.069)	0.325 (0.091)	0.324 (0.067)	0.329 (0.073)	0.490 (0.086)	0.468 (0.082)	0.469 (0.075)
missForest	2.342 (0.467)	2.687 (0.838)	2.423 (0.406)	2.158 (0.645)	2.457 (0.526)	2.511 (0.624)	1.826 (0.351)	1.789 (0.329)	1.844 (0.451)
mean	$10^{-5}(10^{-6})$	$10^{-5}(10^{-6})$	$10^{-5}(10^{-6})$	$10^{-5}(10^{-6})$	$10^{-5}(10^{-6})$	$10^{-5}(10^{-6})$	$10^{-5}(10^{-5})$	$10^{-5}(10^{-6})$	$10^{-5}(10^{-5})$
deletion	0.067 (0.073)	0.070 (0.085)	0.068 (0.081)	—	—	—	—	—	—

Table 1: Comparison of missSOM to the state of the art on the wines data.

	5%			20%			40%		
	MCAR	MAR	MNAR	MCAR	MAR	MNAR	MCAR	MAR	MNAR
Topographic error									
missSOM	0.352 (0.042)	0.356 (0.035)	0.344 (0.049)	0.319 (0.036)	0.315 (0.039)	0.316 (0.048)	0.281 (0.034)	0.281 (0.042)	0.282 (0.045)
Cottrell	0.347 (0.028)	0.367 (0.039)	0.375 (0.049)	0.312 (0.042)	0.339 (0.057)	0.345 (0.053)	0.299 (0.041)	0.303 (0.076)	0.321 (0.075)
knn	0.356 (0.042)	0.359 (0.037)	0.366 (0.045)	0.355 (0.049)	0.360 (0.049)	0.348 (0.053)	0.334 (0.043)	0.360 (0.047)	0.363 (0.049)
missForest	0.346 (0.034)	0.347 (0.047)	0.353 (0.055)	0.351 (0.048)	0.360 (0.056)	0.353 (0.050)	0.339 (0.046)	0.341 (0.063)	0.316 (0.049)
mean	0.362 (0.034)	0.354 (0.046)	0.359 (0.032)	0.361 (0.026)	0.351 (0.037)	0.350 (0.043)	0.345 (0.036)	0.324 (0.038)	0.323 (0.037)
deletion	0.356 (0.041)	0.344 (0.069)	0.315 (0.066)	0.343 (0.063)	0.296 (0.076)	0.344 (0.109)	0.309 (0.050)	0.333 (0.118)	0.272 (0.086)
Quantization error									
missSOM	0.410 (0.149)	0.411 (0.144)	0.406 (0.139)	0.357 (0.122)	0.337 (0.109)	0.348 (0.116)	0.261 (0.085)	0.255 (0.075)	0.258 (0.078)
Cottrell	0.397 (0.140)	0.394 (0.139)	0.391 (0.139)	0.299 (0.099)	0.290 (0.089)	0.305 (0.107)	0.179 (0.054)	0.182 (0.059)	0.187 (0.063)
knn	0.414 (0.149)	0.415 (0.150)	0.410 (0.145)	0.366 (0.129)	0.363 (0.130)	0.363 (0.131)	0.299 (0.105)	0.305 (0.113)	0.288 (0.098)
missForest	0.413 (0.153)	0.413 (0.149)	0.410 (0.154)	0.355 (0.124)	0.343 (0.118)	0.354 (0.126)	0.269 (0.087)	0.276 (0.091)	0.275 (0.096)
mean	0.488 (0.148)	0.469 (0.157)	0.476 (0.145)	0.538 (0.122)	0.480 (0.114)	0.501 (0.117)	0.478 (0.092)	0.416 (0.088)	0.415 (0.078)
deletion	0.396 (0.144)	0.421 (0.152)	0.412 (0.147)	0.315 (0.105)	0.396 (0.137)	0.374 (0.134)	0.224 (0.072)	0.466 (0.163)	0.387 (0.133)
Imputation error									
missSOM	0.617 (0.095)	0.628 (0.097)	0.654 (0.107)	0.671 (0.089)	0.704 (0.083)	0.744 (0.079)	0.746 (0.070)	0.788 (0.070)	0.847 (0.069)
Cottrell	0.596 (0.131)	0.601 (0.135)	0.630 (0.161)	0.645 (0.133)	0.679 (0.130)	0.734 (0.120)	0.765 (0.117)	0.813 (0.112)	0.861 (0.108)
Amelia	0.697 (0.091)	0.711 (0.092)	0.753 (0.111)	0.750 (0.085)	0.782 (0.082)	0.825 (0.081)	0.822 (0.069)	0.874 (0.064)	0.923 (0.074)
knn	0.566 (0.130)	0.569 (0.135)	0.581 (0.158)	0.625 (0.129)	0.623 (0.137)	0.627 (0.135)	0.738 (0.111)	0.735 (0.125)	0.754 (0.135)
missForest	0.519 (0.116)	0.532 (0.116)	0.548 (0.139)	0.579 (0.121)	0.603 (0.116)	0.622 (0.116)	0.712 (0.100)	0.738 (0.100)	0.754 (0.109)
mean	1.005 (0.021)	0.975 (0.071)	1.006 (0.079)	0.998 (0.008)	0.993 (0.066)	1.027 (0.048)	0.999 (0.006)	1.019 (0.045)	1.050 (0.038)
deletion	0.583 (0.132)	0.597 (0.138)	0.628 (0.155)	0.642 (0.136)	0.699 (0.139)	0.791 (0.136)	0.750 (0.117)	0.918 (0.133)	1.022 (0.129)
ARI									
missSOM	0.922 (0.084)	0.924 (0.083)	0.912 (0.091)	0.846 (0.090)	0.825 (0.094)	0.818 (0.077)	0.653 (0.079)	0.611 (0.113)	0.579 (0.093)
Cottrell	0.924 (0.086)	0.923 (0.088)	0.929 (0.081)	0.872 (0.104)	0.864 (0.092)	0.851 (0.084)	0.722 (0.113)	0.688 (0.105)	0.655 (0.091)
kpod	0.886 (0.136)	0.858 (0.149)	0.888 (0.131)	0.758 (0.118)	0.740 (0.172)	0.771 (0.107)	0.496 (0.080)	0.540 (0.093)	0.535 (0.102)
knn	0.921 (0.088)	0.918 (0.094)	0.929 (0.089)	0.892 (0.091)	0.855 (0.161)	0.870 (0.113)	0.767 (0.104)	0.733 (0.108)	0.744 (0.118)
missForest	0.934 (0.077)	0.908 (0.123)	0.912 (0.107)	0.893 (0.091)	0.886 (0.086)	0.865 (0.111)	0.754 (0.105)	0.740 (0.105)	0.735 (0.107)
mean	0.905 (0.094)	0.910 (0.078)	0.903 (0.079)	0.710 (0.105)	0.723 (0.112)	0.722 (0.099)	0.490 (0.073)	0.483 (0.118)	0.478 (0.085)
deletion	0.922 (0.100)	0.929 (0.095)	0.929 (0.087)	0.878 (0.101)	0.849 (0.106)	0.816 (0.108)	0.738 (0.113)	0.588 (0.139)	0.518 (0.124)
Computing time									
missSOM	0.380 (0.004)	0.377 (0.003)	0.386 (0.012)	0.559 (0.004)	0.558 (0.014)	0.546 (0.016)	0.791 (0.009)	0.787 (0.011)	0.792 (0.036)
Cottrell	0.381 (0.002)	0.389 (0.038)	0.387 (0.012)	0.429 (0.008)	0.432 (0.044)	0.418 (0.016)	0.466 (0.013)	0.468 (0.042)	0.466 (0.046)
Amelia	0.194 (0.020)	0.208 (0.039)	0.210 (0.038)	0.212 (0.019)	0.212 (0.016)	0.208 (0.020)	0.227 (0.009)	0.242 (0.013)	0.232 (0.012)
knn	0.571 (0.092)	0.568 (0.076)	0.574 (0.075)	1.956 (0.150)	1.945 (0.174)	1.929 (0.114)	3.284 (0.214)	3.339 (0.228)	3.268 (0.176)
kpod	5.100 (1.753)	4.735 (1.668)	4.874 (1.635)	8.257 (4.370)	7.374 (4.176)	8.444 (3.739)	9.947 (6.487)	14.215 (5.840)	12.042 (9.101)
missForest	30.120 (5.608)	30.745 (6.849)	31.441 (7.084)	28.858 (4.200)	31.242 (4.881)	31.591 (6.128)	23.067 (4.435)	24.017 (5.255)	23.123 (2.939)
mean	10^{-5} (10^{-5})	10^{-5} (10^{-6})	10^{-5} (10^{-6})	10^{-5} (10^{-5})	10^{-4} (10^{-5})	10^{-5} (10^{-5})	10^{-4} (10^{-5})	10^{-4} (10^{-5})	10^{-4} (10^{-5})
deletion	0.315 (0.067)	0.320 (0.069)	0.332 (0.082)	0.192 (0.068)	0.222 (0.088)	0.222 (0.074)	0.162 (0.118)	0.169 (0.059)	0.180 (0.083)

Table 2: Comparison of missSOM to the state of the art on the gaussian mixture data

	5%			20%			40%		
	MCAR	MAR	MNAR	MCAR	MAR	MNAR	MCAR	MAR	MNAR
Topographic error									
basic missSOM	0.337 (0.047)	0.345 (0.035)	0.336 (0.037)	0.313 (0.032)	0.355 (0.063)	0.339 (0.046)	0.294 (0.058)	0.303 (0.057)	0.306 (0.083)
accelerated missSOM	0.352 (0.039)	0.345 (0.049)	0.338 (0.030)	0.301 (0.035)	0.299 (0.039)	0.322 (0.042)	0.282 (0.035)	0.280 (0.059)	0.285 (0.040)
Quantization error									
basic missSOM	0.405 (0.115)	0.394 (0.042)	0.407 (0.145)	0.327 (0.115)	0.326 (0.116)	0.330 (0.112)	0.225 (0.074)	0.233 (0.080)	0.233 (0.077)
accelerated missSOM	0.413 (0.149)	0.408 (0.139)	0.407 (0.138)	0.351 (0.117)	0.340 (0.116)	0.341 (0.115)	0.261 (0.081)	0.245 (0.071)	0.260 (0.074)
Imputation error									
basic missSOM	0.601 (0.140)	0.599 (0.154)	0.613 (0.171)	0.659 (0.125)	0.686 (0.141)	0.759 (0.108)	0.758 (0.093)	0.795 (0.095)	0.871 (0.091)
accelerated missSOM	0.615 (0.097)	0.624 (0.096)	0.654 (0.103)	0.665 (0.092)	0.694 (0.087)	0.750 (0.075)	0.742 (0.069)	0.793 (0.069)	0.848 (0.072)
ARI									
basic missSOM	0.922 (0.092)	0.929 (0.089)	0.937 (0.071)	0.849 (0.088)	0.846 (0.108)	0.823 (0.089)	0.686 (0.108)	0.640 (0.101)	0.623 (0.086)
accelerated missSOM	0.923 (0.090)	0.923 (0.086)	0.922 (0.082)	0.841 (0.092)	0.845 (0.081)	0.805 (0.090)	0.647 (0.094)	0.629 (0.109)	0.591 (0.089)
Computing time									
basic missSOM	33.169 (0.546)	32.940 (0.737)	31.860 (0.396)	33.076 (0.517)	32.988 (0.776)	32.948 (0.530)	33.031 (0.583)	31.920 (0.061)	32.846 (0.0644)
accelerated missSOM	0.394 (0.010)	0.387 (0.006)	0.376 (0.009)	0.557 (0.008)	0.561 (0.017)	0.556 (0.006)	0.790 (0.016)	0.753 (0.011)	0.784 (0.022)

Table 3: Comparison of the basic missSOM Algorithm 2 and its accelerated version Algorithm 3 in terms of different errors and computing time (in seconds).