Imputation in time series

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Abstract
Multivariate time series is a very active topic in the research community and many machine learning tasks are being used in order to extract information from this type of data. However, in real-world problems data has missing values, which may difficult the application of machine learning techniques to extract information. In this paper we focus on the task of imputation of time series. Many imputation methods for time series are based on regression methods. Unfortunately, these methods perform poorly when the variables are categorical. To address this case, we propose a new imputation method based on Expectation Maximization over dynamic Bayesian networks. The approach is assessed with synthetic and real data, and it outperforms several state-of-the-art methods.

1 Introduction

Nowadays the world is full of digital data, due to the large deployment of sensors, fast internet and more computational power to generate all such that data. This data is might be very useful to extract information and predict events, allowing us to control or profit from them. In order to achieve such goal, we need fast algorithms that are capable of finding features that could bring useful information. However, this is a non-trivial task, as data is very large and usual simple statistics are slow and inaccurate. Thus, the term data mining appeared to describe the problem of finding useful information in large data sets by integrating methods from many fields, like machine learning, statistics and database systems, spatial or temporal data analysis, pattern recognition, image and signal processing.

In recent years many works have been done to use machine learning techniques in order to extract useful information from data. The application ranges over several fields, including pharmacokinetics, such as determining clusters of drug absorption [17][6], weather prediction, e.g. find patterns in hurricanes trajectories in order to better forecast the location of a hurricane landfall [10], among others. Currently, with the massive introduction of electronic health records, there is a huge opportunity for mining temporal data with the objective of improving the prediction tasks in the biomedical domain [19].
The main objective of this work is the analysis of multivariate time series, namely, the imputation of missing values. Our approach is to use Dynamic Bayesian Networks, which can represent in a compact way relations between random variables [13]. As such, this work follows the work of [12] and [16] by extending their models. The proposed method is implemented and assessed in synthetic and real data. The real datasets are from UCI Machine Learning Repository [3] and UCR Time Series Classification Archive [1].

Related work

In this paper we only consider the most used methods that support categorical time series, namely the last observation carried forward (LOCF), mode, EM and Amelia. The simplest method is the LOCF, where the missing value is simply imputed as the previous observed value. The Mode imputes the missing value with the most recurrent value. In expectation maximisation (EM) the missing values are considered hidden variables, that are randomly initialized. Then, an EM procedure is performed to improve the distribution of these hidden variables in order to maximize the likelihood of the data. The idea is that the imputed value is the most probable value of the associated hidden variable.

A more complex method is the so called Amelia [8]. This method employs a three-step approach to impute the missing values [14], where the first step creates plausible values for the missing observations. These values are then used to impute the missing values. This process is repeated a number of times, from which it results from the creation of a number of ”complete” datasets. In the second step, these datasets are then analysed using complete-data methods. Finally, the result of the analysis is then combined. In this work we use an R package implementation of Amelia II: A program for missing data as a state-of-the-art imputation method.

2 Background

2.1 Bayesian Networks

Let $X$ be a discrete random variable that takes values over the finite set $\mathcal{X}$. Moreover, let $\mathbf{X} = (X_1, ..., X_n)$ be a $n$-dimensional random vector, where each $X_i$ takes values in $\mathcal{X}_i = \{x_{i1}, ..., x_{ir_i}\}$, where $r_i$ the number of values that $X_i$ can take. A Bayesian Network (BN) is composed of a Directed Acyclic Graph (DAG) that encodes a joint probability distribution over a set of random variables [13].

**Definition 1.** A $n$-dimensional Bayesian Network (BN) is a triple $B = (\mathbf{X}, G, \Theta)$ where:

- $\mathbf{X}$ is an $n$-dimensional finite random vector where each random variable $X_i$ ranges over by a finite domain $D_i$. Henceforward, it is denoted the joint domain by $D = \prod_{i=1}^{n} D_i$. 

• $G = (N, E)$ is a DAG with nodes $N = \{X_1, \ldots, X_n\}$ and edges $E$ representing direct dependencies between variables.

• $\Theta$ encodes the parameters $\{\theta_{ijk}\}_{i \in \{1, \ldots, n\}, j \in D_{\Pi X_i}, k \in D_i}$ of a network, given by:

$$
\theta_{ijk} = P_B(X_i = x_{ik} | \Pi X_i = w_{ij}),
$$

where $\Pi X_i$ denotes the set of parents of the node $X_i$ in the DAG $G$, $x_{ik}$ is the $k$-th values of $X_i$ and $w_{ij}$ is the $j$-th configuration of $\Pi X_i$. Moreover, $q_i$ is the number of total parents configurations of $X_i$, $q_i = \prod_{X_j \in \Pi X_i} r_j$.

Intuitively, the network structure of a DAG $G$ encodes conditional independence assumptions, where each random variable $X_i$ is only dependent of the descendants nodes and independent of its nondecendants, given its parents. These independence assumption are used within the chain rule to provide a factorized joint distribution over $X$, defined as:

$$
P_B(X_1, \ldots, X_n) = \prod_{i=1}^{n} P_B(X_i | \Pi X_i).
$$

(1)

Learning a BN $B = (X, G, \Theta)$ reduces to the problem of finding the network structure $G$ and the parameters $\Theta$ that best fits the data $D$. When data $D$ is complete, i.e. there are no missing values and hidden variables, being $D = \{y_1, \ldots, y_N\}$ given by a set of $N$ i.i.d. instances, usually score-based learning is employed. Therein, a scoring criterion $\phi$ is used to measure how well a candidate network $B$ describes $D$. However, since learning BN is a NP-hard problem, the search space of possible solutions is explored by restring the solution space (tree-like \cite{5} or CκG-like network structures \cite{16} or heuristic methods (greedy-hill climber \cite{7}). In both cases, learning can be stated as an optimization problem:

$$
\max_{B \in \mathcal{B}_n} \phi(B, D),
$$

(2)

where $\mathcal{B}_n$ corresponds to the set of BNs with $n$ variables being searched.

2.2 Dynamic Bayesian Networks

The Dynamic Bayesian Network (DBN) extends the representation of BN to temporal processes. For simplicity, assume the discretization of time in time slices $\{0, \ldots, T\}$. Let $X[t] = (X_1[t], \ldots, X_n[t])$ be a random vector that denotes the values of the set of random variables $X$ over the time $t$. Moreover, let $X[t_1 : t_2]$ denote the set of random vectors $X[t]$ over $t_1 \leq t \leq t_2$. Finally, let the joint probability distribution over the trajectory of a stochastic process from $X[0]$ to $X[T]$, $P(X[0], \ldots, X[T])$, abbreviated with $P(X[0 : T])$, be defined as:

$$
P(X[0 : T]) = P(X[0]) \prod_{t=1}^{T-1} P(X[t + 1] | X[0 : t]).
$$

(3)

One common approach to ease computation is to assume that the process is Markovian in $X$. 

3
Definition 2. A stochastic process is said to satisfy the $m$-th order Markov assumption if, for all $t \geq 0$:
\[
P(X[t+1] | X[0 : t]) = P(X[t+1] | X[t - m + 1 : t]),
\]
where in this case $m$ is called the Markov lag of the process.

Another assumption that simplifies the computation of the joint probability distribution is to consider the process to be stationary. This assumption is usually adequate when the number of time slices in the training data is small.

Definition 3. A Markovian process is said to be stationary if:
\[
P(X[t+1] | X[t]) \text{ is equal for all time slices } t \in \{0, ..., T - 1\}.
\]

Rigorously, a DBN is composed of two networks: an initial BN that encodes dependencies among variables in the initial state $X[0]$, and a transition network that explains how dependencies flow forward in time. These dependencies include the intra-slice (from $X[t]$ to $X[t + 1]$) and inter-slide (among $X[t + 1]$) dependencies.

Definition 4. A stationary first-order Markov DBN consists of:
- A prior network $B^0$, which specifies the distribution over the initial states $X[0]$;
- A transition network $B_t^{t+1}$ over the variables $X[t] \cup X[t+1]$, for all $t$, that specifies the transition probability $P(X[t+1] | X[t])$.

An example of a DBN along with its unrolled network for three time-slices is depicted in Figure 1.

![Figure 1: Example of a stationary first-order Markov DBN.](image)

In the case that all data is observed, there are three approaches for learning dynamic Bayesian networks. The first approach learns optimal DBN using mutual information tests, but ignores intra-slice dependencies. A polynomial-time algorithm that learns an optimal DBN can address both inter and intra-slice connections,
a polynomial-time algorithm was recently proposed [12]. However, to keep the complexity low, the search space for the intra-slice connections is restricted to tree augmented networks, i.e., acyclic networks where each variable has only one parent from the same time slice, but can have a finite number of parents from the previous time slices. The resultant network is denoted by tDBN. More recently, the search space was extended exponentially [15, 16] to networks where the intra-slice network has in-degree at most $\kappa$ and is consistent with the Breadth-First Search (BFS) order of the tDBN. The resultant network of this method is denoted by bcDBN.

3 Structural EM

In many cases, the assumption that the training data are fully observed is simply unrealistic. Since this assumption is crucial for learning the structure and the parameters of a BN some changes to the learning process need to be made. When data $D$ is incomplete due to missing values or hidden variables, however, scoring functions are no longer decomposable. This shortcoming was addressed in [5], where the Structural Expectation-Maximization (SEM) iterative method to learn a BN with hidden variables and/or missing values, a brief description of this method can be seen in this section.

3.1 Parameter Estimation

The first learning task that will be considered is the parameter estimation task. As in the case of the complete data, the approach that will be used is the Maximum Likelihood Estimation (MLE). So given a network structure $G$ and the form of the Conditional Probability Distributions (CPDs), it is only necessary to compute the parameters $\Theta$ to define the distribution $P(X \mid \Theta)$. It is also given a data set $D$ that consists of $M$ partial instances of $X$, so it is needed to compute the values $\hat{\Theta}$ that maximize the log-likelihood function:

$$\hat{\Theta} = \arg \max_{\Theta} \log L(\Theta : D).$$

(6)

Unlike the complete data case, where sufficient statistics are collected for each CPD allowing to compute the parameters that maximize the likelihood, in the case of missing data there is no access to full sufficient statistics. In order to have access to them, one can take a simple approach of filling the missing values arbitrarily. Some strategies to fill these missing values consist on choosing some default value or one according to some prior distribution. The problem with this approach is that the filled value will introduce bias in the learned parameters.

Another approach tries to solve two different problems at once, these problems being the learning of the parameters and imputation of the missing values. To be noted that each of these tasks is very easy when the solution to the other is present.
The Expectation Maximization (EM) algorithm starts by choosing some arbitrary starting point. This can be either a choice of parameters or some assignment to the missing values. Assuming that it begins with a parameter assignment, then the algorithms repeat two steps. The first step is to use the current parameters in order to complete the data, using probabilistic inference. The second step, consists in using the completed data as if it was observed and compute a new set of parameters. So, given a set of parameters $\theta^0$ and a partial instance, the posterior of all possible assignments to the missing value of that instance can be calculated. The EM algorithm then uses this probabilistic completion of different data instances to estimate the expected value of the sufficient statistics. It is well known that each iteration of this method increases the log-likelihood (see for instance [9]), and moreover, that this process converges to a local maximum of the likelihood function.

It is worthwhile to give a more detailed explanation of the EM algorithm. Assume the general BN with table-CPDs and an initial assignment for the parameters $\Theta^0$. Let $X$ be all the child variables, $W$ all the parent variables and $o$ the dataset composed by $M$ data instances. The algorithm iterates over the following steps.

**Expectation (E-Step)** In this step the Expected Sufficient Statistics (ESS) are computed, this is done by using the current parameters $\Theta^t$.

- For each family $X$, $W$ and for each data case $o[m]$, compute the joint probability $P(X,W \mid o[m], \Theta^t)$.
- Compute the ESS for each $x$, $w$,
  \[
  \bar{M}_{\theta^t}[x, w] = \sum_m P(x, w \mid o[m], \theta^t).
  \]

**Maximization (M-Step)** Given the ESS, it performs maximum likelihood estimation, with respect to them, in order to compute a new set of parameters,

\[
\theta^{t+1}_{x \mid w} = \frac{\bar{M}_{\theta^t}[x, w]}{\bar{M}_{\theta^t}[w]}.
\]

In Algorithm 1 and Algorithm 2 the E-Step and for the Parameter EM are given.

### 3.2 Structure Learning

The intuition behind Structural EM algorithm is the same that was applied to solve the problem of learning the parameters of a BN when there is missing data. Like the parameter estimation, there is two main steps, the expectation, where a complete data set is generated, and a maximisation, where the network structure is learned. The main difference between the Structural Expectation-Maximization (SEM) and the parameter estimation is that the maximisation...
Algorithm 1 Compute the expected sufficient statistics

1: **procedure** `Compute-ESS(G, Θ, D)`
2:   **for** each $i = 1, \ldots, n$ do  \texttt{▷} Initialization of data structures
3:     **for** each $x_i, w_i \in Val(X_i, \Pi^G_{X_i})$ do
4:         $M_t[x_i, w_i] \leftarrow 0$
5:   **for** each $m = 1, \ldots, M$ do \texttt{▷ Collect probabilities from all instances}
6:       Run inference on $(G, Θ)$ using evidence $o[m]$
7:   **for** each $i = 1, \ldots, n$ do
8:       **for** each $x_i, w_i \in Val(X_i, \Pi^G_{X_i})$ do
9:           $\bar{M}_t[x_i, w_i] \leftarrow \bar{M}_t[x_i, w_i] + P(x_i, w_i | o[m])$
10:      **return** $\{M_t[x_i, w_i] : \forall i = 1, \ldots, n, \forall x_i, w_i \in Val(X_i, \Pi^G_{X_i})\}$

Algorithm 2 Expectation-Maximization algorithm for Bayesian Network(using table-CPDs)

1: **procedure** `Expectation-Maximization(G, Θ^0, D)`
2:   **for** each $t = 0, \ldots$, until convergence do
3:       $\{M_t[x_i, w_i]\} \leftarrow \text{Compute-ESS}(G, \Theta^t, D)$ \texttt{▷ E Step}
4:   **for** each $i = 1, \ldots, n$ do \texttt{▷ M Step}
5:       **for** each $x_i, w_i \in Val(X_i, \Pi^G_{X_i})$ do
6:           $\theta^t_{x_i|w_i} \leftarrow \frac{M_t[x_i, w_i]}{M_t[w_i]}$
7:   **return** $\Theta^t$
step, in the Structural Expectation-Maximization (SEM), besides learning the parameters, the network structure is also learned. Moreover, [9] state that by using the Minimum Description Length (MDL) score it is guaranteed that, in each iteration, the learned structure is better than the one used in the previous iteration. From this statement, it results that the SEM algorithm will monotonically improve the score. The pseudo-code of the algorithm is given in Algorithm [3].

Algorithm 3 Structural EM algorithm for Bayesian Networks

1: procedure STRUCTURAL-EM($G^0, \Theta^0, D$)
2:   for each $t = 0, \cdots$, until convergence do
3:     $\Theta^t' \leftarrow$ Expectation-Maximization($G^t, \Theta^t, D$) \triangleright Optional parameter learning step
4:     $G^{t+1} \leftarrow$ Structure-Learn($D_{G^t, \Theta^t'}$) \triangleright Run EM to generate the ESS for $D_{G^t, \Theta^t'}$
5:     $\Theta^{t+1} \leftarrow$ Estimate-Parameters($D_{G^t, \Theta^t'}, G^{t+1}$)
6: return $G^t, \Theta^t$

4 Proposed Method

One common problem with multivariate time series is missing values. Mostly because many methods assume full data and are useless in this scenario. Thus, finding ways to work with missing values becomes crucial. One of the most used approaches to solve this problem is to drop the observations with missing values, however, when the dataset has few observations this approach can lead to enormous loss of information.

Another approach that one can take is to impute the missing values. In this approach, the missing values are “filled” using some method, like an interpolation. Since the focus of this thesis is the multivariate categorical time series, the most common methods for interpolation does not apply. So in order to impute the missing values, this work proposes a method that uses the SEM algorithm, devised by [4], to learn the structure of the data with missing values. However, because the algorithm learns BNs, it cannot model a time series, as such the algorithm was changed for the purpose of learning DBNs. As before, the search space is restricted to tDBN [12] and bcDBN [16]. The SEM algorithm can be divided with two big steps the parameter learning and the structure learning, and because the dataset has missing values one step cannot be learned without the other. As such, this algorithm starts by generating a DBN randomly. Then the “true” parameters of the fixed network can be learned. This is done in an iterative process where first the ESS are computed and then the new set of parameters are computed. This is done until convergence. With the parameters learned the algorithm then learns a new structure and repeats this process until the convergence criterion is met.
Finally with the DBN given by the SEM, the imputation algorithm then generate again a new dataset without missing values, however instead of having all the possible combinations of values that could fill the missing values, this dataset fills the missing values with the combinations that maximizes the posterior probability. In section 3 can be seen a description of the SEM algorithm which will be the base to develop the imputation algorithm.

Algorithm 4 Missing values imputation via a DBN

1: procedure IMPUTATION-DBN(D)
2: \( G^0, \Theta^0 \leftarrow \) Generate a random DBN
3: \( G, \Theta \leftarrow \) Structural-EM\((G^0, \Theta^0, D)\)
4: for each observation in \( D \) do
5: \hspace{1em} for each transition in the observation do
6: \hspace{2em} if transition has missing values then
7: \hspace{3em} Generate all possible combinations of values for the missing values
8: \hspace{2em} for each new combination of values do
9: \hspace{3em} Calculate the posterior probability
10: \hspace{3em} Select the generated combination that maximizes the posterior probability and impute the missing values
11: \hspace{1em} Add the observation to \( D' \)
12: return \( D' \)

5 Experimental Results

5.1 Simulated data

To assess the merits of the SEM algorithm as an imputation method, multivariate time series were randomly generated using generated DBNs. Then various datasets were generated, where the characteristics like the number of observations and the number of variables were changed. Finally, the missing values were generated with respect to two parameters, the first is the percentage of subjects with missing values and the second is the percentage of missing values corresponding to a subject. With the purpose of comparing this imputation method with state of the art methods, first these methods were used to impute the datasets with missing values, then the number of errors between the original dataset, without missing values, and the imputed datasets were counted. To facilitate the visualization, the results of this experiments are grouped in Figure 2.

When analysing the results presented in Figure 2, it can be concluded that the imputation done by SEM algorithm has fewer errors when comparing with other imputation methods like Last Observation Carried Forward (LOCF), Mode and the Amelia [8]. This result was expected because the data were generated using DBNs, however, it important to highlight that despite the SEM algorithm has
fewer errors, it has errors. One justification of this can be the fact that the
imputation chosen by the algorithm is the one that maximizes the probability
of the observation.

5.2 Benchmark data

In order to evaluate the performance of the SEM algorithm as an imputation
method it was used 10 datasets from UCI Machine Learning Repository [3] and
UCR Time Series Classification Archive [1]. Moreover, because the implement-
ation of the SEM algorithm only works with categorical time series and most
of these datasets are composed by real-valued time series a discretization of
these time series must be done. The discretization was done using the SAX
algorithm [11], it is important to note that it was used only an alphabet size
of four, a maximum size of the time series of one hundred time steps and an
independently discretization of each dimension of multivariate time series
.

With the resulting discretized datasets, in order to test the performance of
the imputation methods, it was removed values. Once more, these values were
removed with respect to two parameters, the percentage of observation with
missing values and the percentage of missing values per missing observation.

Moreover, in order to use the SEM algorithm some assumptions need to be
made, these are the stationarity of the time series and the first-order Markov
assumption. Analysing the results, Figure 4, it can be concluded that, in most
datasets, the imputation done with SEM algorithm has fewer errors than the
other methods.

Given these results, a Wilcoxon signed ranks test was performed, in order
to compare the SEM algorithm with others imputation methods. As such, the
results were grouped by methods and by the percentage of observations with
missing values, Table 1. The use of a Wilcoxon signed ranks test is justified by
the fact that is simple and a robust non-parametric test for statistical compar-
isons [2].

When analysing results from Table 1 it is easy to note that almost all p-
values have a value below 0.05, which indicates that the null-hypothesis, that
the two algorithms perform equally well, is discarded. However, it is important
to note that the imputation errors of LOCF are similar to the imputation errors
of the SEM algorithm which is a strange result. One explanation for this result
Figure 3: Imputation errors for real datasets.

| Method | 10     | 20     | 30     | 40     |
|--------|--------|--------|--------|--------|
| LOCF   | 1.74E-02 | 1.25E-02 | 3.22E-02 | 1.26E-01 |
| Mode   | 5.89E-03 | 1.95E-03 | 1.95E-03 | 1.95E-03 |
| Amelia | 1.95E-03 | 1.95E-03 | 1.95E-03 | 1.95E-03 |

Table 1: Results from the Wilcoxon signed ranks test between SEM algorithm and other methods.

can be the number of symbols used to discretize the time series, because since 4 symbols were used the discretized time series may not vary that much over time, which leads to a lower imputation error when using the LOCF.

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Figure 4: Imputation errors for real datasets.

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