Automatic interpretation of classes for improving decision support

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Abstract: More and more, the analysis of clustering results becomes difficult as the number of variables considered increases, and the number of classes is not low. Sometimes concept induction methods are used to associate concepts to every class and use to be expressed as boolean expressions, easy to understand and supposedly providing good support to decision making. It has been seen that most of the concept induction algorithms prioritize the compacity of the final expressions, as well as their predictive power. However, for descriptive purposes, when the meaning of classes has to be recognized and understood by the expert, this is not the best approach, since compacity directly implies elimination of redundancies or strong associations, while comprehension of the class is mainly based in understanding how variables interact among them inside the class. Here a method to induce conceptual descriptions of classes is proposed, providing non-minimal descriptions of the classes, but richer ones including the characteristics that distinguishes a class from the others, in such a way that expert can easily recognize the essence of the class, and conceptualize it on the bases of local interactions among all variables observed inside every class. This kind of interpretations provide an excellent support for later decision support systems.

Keywords: Knowledge Discovery and Data Mining; Hierarchical clustering; class interpretation; Induction rules; Waste Water treatment plants.

1 Introduction

In automatic classification where the classes composing a certain domain are to be discovered, one of the most important required processes and one of the less standardized, is the interpretation of the classes (Gordon [1994]), closely related with validation Volle [1985.], and critical in the later usefulness of the discovered knowledge. The interpretation of the classes, so important to understand the meaning of the obtained classification as well as the structure of the domain, used to be done in an artistic-like way Hand [1996]. But this process becomes more and more complicated as the number of classes grows. This work is involved with the automatic generation of useful interpretations of classes in such a way that decisions about the action associated to a new object can be modeled and it is oriented to develop, in the long term, intelligent decision support systems.

The presented proposal integrates different findings from a series of previous works: Pérez-Bonilla and Gibert [2007] proposed a single methodological tool which takes advantage of the hierarchical structure of the clustering to overcome some of the limitations observed in Gibert et al. [1998], Gibert [1996]. In the present work, for the first time, the whole proposal, named Conceptual Characterization by Embedded Conditioning (CCEC), is applied to a real environmental data set and different possibilities for integrating knowledge from one iteration to the
following one are exhaustively compared and evaluated. For the first time this work presents a depth analysis of the quality of the solutions provided by 5 different strategies, both considering structural quality criteria, as confidence or support of the provided descriptions as well as more semantic criteria, as the proximity towards the descriptions provided by the experts.

This paper is organized as follows: After the introduction, the methodology is presented in §2. §3 introduces the waste water treatment plant (WWTP) of the case study and the data used. Results of applying CCEC to the data described are given in §4. Finally in §5 the conclusions and the future work are addressed.

2 FORMAL FRAME

The standard input of a clustering algorithm is a data matrix with the values of $K$ variables $X_1, \ldots, X_K$ (numerical or not) observed over a set $I = \{1, \ldots, n\}$ of individuals. Variables are in columns, while individuals in rows. Cells contain the value $(x_{ik})$, taken by individual $i \in I$ for variable $X_k, \{k = 1 : K\}$. The set of values of $X_k$ is named $D^k = \{c^k_1, c^k_2, \ldots, c^k_s\}$ for categorial variables and $D^k = r_k$ for numerical ones, being $r_k = [\min X_k, \max X_k]$ the range of $X_K$. A partition in $\xi$ classes of $I$ is denoted by $\mathcal{P}_\xi = \{C_1, \ldots, C_\xi\}$, and $\tau = \{P_1, P_2, P_3, \ldots, P_n\}$ is an indexed hierarchy of $I$. Finally, $\mathcal{P}_2 = \{C_1, C_2\}$ is a binary partition of $I$. Usually, $\tau$ is the result of a hierarchical clustering over $I$, and it can be represented in a graphical way as an horizontal cut of the corresponding dendrogram (or hierarchical tree, see Figure 1, Pérez-Bonilla et al. [2008]).

CCEC is a methodology globally described in Pérez-Bonilla et al. [2008] that takes advantage of the existence of $\tau$ to generate conceptual interpretations of a of a given partition $\mathcal{P} \in \tau$ in terms of formal descriptions. CCEC uses the property of all binary hierarchical structure that $\mathcal{P}_{\xi + 1}$ has the same classes of $\mathcal{P}_\xi$ except one, which splits in two subclasses in $\mathcal{P}_{\xi + 1}$. The binary hierarchical structure represented in $\tau$ is used in CCEC to discover particularities of the final classes step by step by analyzing the hierarchy top-down. It uses Boxplot based discretization (BBD), see Gibert and Pérez-Bonilla [2006]), as an efficient way of transforming all numerical variable into qualitative ones in such a way that every resulting qualitative variable maximizes the association with the reference partition. See Gibert and Pérez-Bonilla [2006] for details. Briefly, main idea is to use as cut-points the extreme values (minimum and maximum) that the numerical variable locally takes in every class of $\mathcal{P}$. BBD is the kernel of Boxplot based induction rules (BbIR) (presented in Pérez-Bonilla and Gibert [2007]). It is a method for inducing probabilistic rules ($r : x_{ik} \in I^k \stackrel{E_{sc}}{\longrightarrow} C$, being $p_{sc} \in [0, 1]$ the certainty degree of $r$). The produced rules have a minimum number of attributes in the antecedent, and those are formalized on the basis of the intervals induced by BbD for every variable. The CCEC methodology was formalized in Pérez-Bonilla et al. [2008]. Here an algorithmic version is presented:

1. Consider the top of the tree: $\xi = 1$; $\mathcal{P}_1 = I$; $\mathcal{A}_{\mathcal{P}_1} = \{A^1 : true\}$
2. Go down one level in the tree, by making $\xi = \xi + 1$ and so considering the new $\mathcal{P}^\xi$. Being $\tau$ an indexed hierarchy, $\mathcal{P}^\xi$ is embedded in $\mathcal{P}^{\xi - 1}$ in such a way that there is a single class of $\mathcal{P}^{\xi - 1}$, namely $C^\xi_1$, splitting in two new classes of $\mathcal{P}^\xi$, namely $C^\xi_1$ and $C^\xi_2$ and all other classes $C^\xi_q, q \neq i, j$, are common to both partitions and $C^\xi_q = C^{\xi - 1}_q \forall q \neq i, j$. Consider the restricted partition $\mathcal{P}^*_\xi = \{C^\xi_1, C^\xi_2\}$. It holds that $\mathcal{P}^*_\xi \subset \mathcal{P}^\xi$ and when $\xi = 2$, $\mathcal{P}^*_\xi = \mathcal{P}^\xi$. As in previous iteration the class $C^{\xi - 1}_1 = \{C^\xi_1 \land C^\xi_2\}$ was already distinguished from the rest by proper concept, it is enough to find distinction between $C^\xi_1$ and $C^\xi_2$. 

![Figure 1: Dendrogram](image-url)
3. Use BbD (Gibert and Pérez-Bonilla [2006]), to find (total or partial) characteristic values regarding \( P_\xi = \) Gibert et al. [1998] for all numerical variables.

4. Use BbIR, to induce a knowledge base \( R(P_\xi) \) describing both classes \( \{ C_1^\xi, C_2^\xi \} \).

5. Search the best rule for each class of the restricted partition \( P_\xi = \{ C_1^\xi, C_2^\xi \} \). In the next section several criteria are presented to determine them. Name \( A_1^\xi \) and \( A_2^\xi \) the antecedents of the rules selected for \( C_1^\xi \) and \( C_2^\xi \) respectively.

6. Integrate \( A_1^\xi \) and \( A_2^\xi \) with the father’s concept from previous iteration. Compound concepts are associated to \( C_1^\xi \) and \( C_2^\xi \):

\[
A_1^\xi = A_1^{\xi-1} \land A_1^\xi ; \quad A_2^\xi = A_2^{\xi-1} \land A_2^\xi
\]

(1)

Description of both \( C_1^\xi \) and \( C_2^\xi \) inherits the properties of the father class \( C_t^{\xi-1} \).

7. Build the concepts system:

\[
A_P_\xi = A_{P_{\xi-1}} \setminus \{ C_t : A_t \} \cup \{ C_1^\xi : A_1^\xi, C_2^\xi : A_2^\xi \}
\]

8. Go down one level in the tree, by making \( \xi = \xi + 1 \) and so considering \( P^{\xi+1} \). Return to step 2 and repeat until \( P^\xi = P \). Target partition to be interpreted.

9. Finally, \( A_P_\xi = \{ C : A_C \ \forall C \in P_\xi \} \) and also, the concepts system can be associated to a rules system \( R(P^\xi) = \{ r tq r : A \rightarrow C \ \forall C \in P_\xi \} \).

The set of concepts \( A_P_\xi \) can, in fact, be considered as a domain model which can support later decision-making Power [2002] on the application domain. As a standard treatment is previously associated to every class by experts, evaluation of \( A_P_\xi \) on new objects can help for treatment assignment. In this context, the possibility of easily interpreting and understanding the classes is critical. The proposed method provides simple and short rules which use to be easier to handle than those provided by other inductive methods.

### 2.1 Finding best concept at every iteration

The quality of a single rule \( r : A_C(i) \rightarrow C \) is evaluated according to 3 criteria:

- **Support (Sup):** is the proportion of objects in \( I \) that satisfy the antecedent of the rule, Liu et al. [2000]. \( \text{Sup}(r) = \frac{\text{card}(i \in I \land A_C(i) = \text{true})}{n} \). It measures the popularity of a rule.

- **Relative covering (CovR):** is the proportion of objects in class \( C \) that satisfy the antecedent of rule. \( \text{CovR}(r) = \frac{\text{card}(i \in C \land A_C(i) = \text{true})}{n_C} \). It measures the coverage of the rule inside a certain class.

- **Confidence (p(r)):** proportion of objects in the antecedent \( (A_C(i) = \text{true}) \) that belong to \( C \), Liu et al. [2000]. \( p(r) = \frac{\text{card}(i \in C \land A_C(i) = \text{true})}{\text{card}(A_C(i) = \text{true})} \). It measures the correctness of \( r \).

The quality of a Knowledge Base is evaluated according to 3 summarizing criteria:

- **Average confidence:** \( p(R) = \frac{\sum_{r \in R} \text{Sup}(r) \cdot p(r)}{n_R} = \frac{\sum_{r \in R} \frac{\text{card}(i \in C \land A_C(i) = \text{true})}{n_C}}{n_R} \)

- **Total Support:** \( \text{Sup}(R) = \sum_{r \in R} \text{Sup}(r) = \sum_{r \in R} \frac{\text{card}(i \in C \land A_C(i) = \text{true})}{n_C} \)

- **Global covering:** \( \text{Cov}_{\text{global}}(R) = \sum_{C \in C} \frac{\text{card}(i \in C \land A_C(i) = \text{true}) \times n_C}{n} \)

Five different methods of selecting best concepts and combining with the knowledge of previous iteration are considered:
Best Global concept and Close-World Assumption (BG &CWA): Restrict the search to the set of certain rules \( p(r)=1 \) \( S(P_{\xi+1}^*) \subseteq S(R_{\xi+1}^*) \). Choose the rule that maximizes the relative covering in \( S(P_{\xi+1}^*) \). Use a Close-World Assumption (CWA) to conceptualize the complementary class by means of the negation of selected concept.

Best local concept and no Close-World Assumption (BL &noCWA): Choose the rule that maximizes the relative covering inside \( S_{C_i}(P_{\xi+1}^*) = \{ r \in S(P_{\xi+1}^*) \mid r : A_C(i) \rightarrow C_i \} \) and \( S_{C_j}(P_{\xi+1}^*) = \{ r \in S(P_{\xi+1}^*) \mid r : A_C(i) \rightarrow C_j \} \).

Best local concept and Close-World Assumption (BL &CWA): Choose the rule that maximizes the relative covering in both \( S_{C_i}(P_{\xi+1}^*) \) and \( S_{C_j}(P_{\xi+1}^*) \). Use a CWA to add the negation of the concept selected for the complementary class.

Best local concept and partial Close-World Assumption (BL &partial-CWA): Includes the same concepts as the BL local concept and CWA except when the selected concept refers to the same variable for the two classes. In this case the original concept is kept.

Best local-global concept and Close-World Assumption (BL+G &CWA): Includes the same variables as the BL &partial-CWA except when the selected concepts refers the same variable for both classes. In this case the best concept is kept and the negation is added to the complementary class.

3 Case study

A case study in this paper was the pilot plant, located in Domđale-Kamnik waste water treatment plant in Slovenia. A scheme of the pilot plant with sensors and actuators is shown in Figure 2. In the pilot plant the moving bed biofilm reactor (MBBR) technology is tested for the purpose of upgrading the whole plant for nitrification and denitrification. The pilot plant with the volume of 1125 m\(^3\) consists of two anoxic and two aerobic tanks that are filled with the plastic carriers on which the biomass develops, a fifth tank, which is a dead zone without plastic carriers and a settler. The total air flow to both aerobic tanks can be on-line manipulated in such a way that oxygen concentration in the first aerobic tank is controlled at the desired value. The waste water rich with nitrate is recycled with the constant flow rate from the fifth tank back to the first tank. The influent to the pilot plant is waste water after mechanical treatment, which is pumped to the pilot plant. The inflow is kept constant to fix the hydraulic retention time. The influent flow rate can be adjusted manually to observe the plant performance at different hydraulic retention times. The database used in this study consists of 365 daily averaged observations from the 1st of June 2005 to the 31th of May 2006. Every observation includes measurements of the 16 variables that are relevant for the operation of the pilot plant. The variables are:

- NH\(_4\)-influent: ammonia concentration at the influent of the pilot plant(pp) (3 in Fig. 2).
- Q-influent: waste water influent flow rate of the pp (7 in Fig. 2).
- TN-influent: concentration of the total nitrogen at the influent of the pp (4 in Fig. 2).
- TOC-influent: total organic carbon concentration at the influent of the pp (5 in Fig. 2).
- Nitritox-influent: measurement of the inhibition at the influent of the pp (6 in Fig. 2).
- h-waste water: height of the waste water in the tank (no in Fig. 2).
- O\(_2\)-1aerobic: dissolved oxygen concentration in the 1st aerobic tank (3rd tank) (12-Fig. 2).
- Valve-air: openness of the air valve (0-100%), highly related with Q-air (V2 in Fig. 2).
- Q-air: total air flow that is dosed in both aerobic tanks (1 in Fig. 2).
- NH\(_4\)-2aerobic: ammonia concentration in the second aerobic tank (9 in Fig. 2).
- O\(_2\)-2aerobic: dissolved oxygen concentration in the 2nd aerobic tank (4th tank) (13-Fig. 2).
- TN-effluent: concentration of the total nitrogen at the effluent of the pp (no in Fig. 2).
- Temp-waste water: temperature of the waste water (14 in Fig. 2).
- TOC-effluent: total organic carbon concentration at the effluent of the pp (no in Fig. 2).
- Freq-rec: frequency of the internal recycle flow rate meter (no in Fig. 2).
- FR1-DOTOK-20s (Hz): frequency of the motor that pumps the waste water into the plant.
The data base was clustered in a previous work in order to identify typical situations that could improve decision making, since managing WWTP is difficult in general and requires great expertise. See Metcalf and Eddy [2003] for details on the problematics related with management and control of WWTP and the difficulties of finding global mechanistic models. In Gibert [1996] clustering based on rules was used with the following Knowledge Base:

\[ KB = \{ r_1 : ( (\text{and}(\geq (\text{NH}_4 - 2\text{aerobic})10.0))(> (\text{TN} - \text{effluent})18.0)) \rightarrow \text{Mmonia}) , \\
    r_2 : ( (\text{and}(< (\text{NH}_4 - 2\text{aerobic})10.0))(> (\text{TN} - \text{effluent})18.0)) \rightarrow \text{Nitrogen}) \} \]

with 38 objects satisfying \( r_1 \), 80 objects satisfying \( r_2 \) and the final dendrogram of Figure 1 (see details in Pérez-Bonilla et al. [2008]). A final partition in 4 classes was \( P_4 = \{ C_{353}, C_{357}, C_{358}, C_{360} \} \) is obtained. Experts provided the following interpretation:

- \( C_{353} \) represents the plant operation under the high load. In this case influent nitrogen concentrations are high and also influent flow rate is quite high as well. Even though the oxygen concentration in the aerobic tanks are high this can not decrease the effluent nitrogen concentrations. It means that, when the plant is overloaded, high effluent concentrations at the effluent can be expected.
- \( C_{357} \) represents the situation when the influent flow rate is low, that is, when the hydraulic retention time of the plant is high. In this case, as oxygen concentration in the aerobic tank is high enough, quite low effluent nitrogen concentrations can be obtained. In front of low influent flow rate, the effluent concentrations can be low if the oxygen concentration in the aerobic tanks is high.
- \( C_{358} \) explains the situation when the waste water temperature is low. In this case nitrogen removal efficiency of the plant is rather low. This happens because microorganisms in the tanks do not work so intensively in cold conditions and therefore higher concentrations at the effluent can be expected.
- \( C_{360} \) shows the situation when the waste water temperature is high. In warmer conditions the microorganisms in the plant work faster, so the effluent nitrogen concentrations can be low even when the oxygen concentrations in the aerobic tanks are quite low.

Figure 2: MBBR (Moving Bed Biofilm Reactor) pilot plant with sensors and actuators.

4 RESULTS

In this section CCEC has been applied to the data of the plant by testing the 5 aggregation criteria presented before and compared with the interpretation provided by the experts from scratch. The descriptions obtained for every class with the different methods are shown in Table 3. Results for intermediate iterations are presented in Pérez-Bonilla et al. [2008]. Table 1 shows quality indicators of the results (Confidence, Support and Coverage). The method that gives the most similar interpretation to those provided by the expert is the Best Local-Global and Close World Assumption (BL+G & CWA), which from a technical point of view also seems to represent the more equilibrated option with the second higher values in both global coverage and support. The greatest Global coverage is from Best Local and Close World Assumption, but this interpretation is redundant. So the best interpretation is the one obtained using BL+G & CWA.

5 CONCLUSIONS AND FUTURE WORK

In this paper a methodology to generate automatic conceptual interpretations of a group of classes is presented. Concepts associated with classes are built taking advantage of hierarchical structure of the underlying clustering. The Conceptual characterization by embedded conditioning Pérez-Bonilla and Gibert [2007], is a quick and effective method that generates a conceptual model of the domain, which will be of great support to the later decision making based on a combination
Best global concept and Close-World assumption:

\[ R(P_4) = \{ \text{Valve-\textit{air},i} \in [54.777, 69.898] \land \text{xInfuent,i} \in [28.792, 83.792] \land \text{xTemp-\textit{ww},i} \in [8.427, 13.327] \land \text{xTemp-\textit{ww},i} \in [3.327, 21.896] \} \]

Best local concept and Close-World assumption:

\[ R(P_4) = \{ \text{Valve-\textit{air},i} \in [54.777, 69.898] \land \text{xInfuent,i} \in [28.792, 83.792] \land \text{xTemp-\textit{ww},i} \in [8.427, 13.327] \land \text{xTemp-\textit{ww},i} \in [3.327, 21.896] \} \]

Best local concept and no Close-World assumption:

\[ R(P_4) = \{ \text{Valve-\textit{air},i} \in [54.777, 69.898] \land \text{xInfuent,i} \in [28.792, 83.792] \land \text{xTemp-\textit{ww},i} \in [8.427, 13.327] \land \text{xTemp-\textit{ww},i} \in [3.327, 21.896] \} \]

Best Local-Global concept and Close-World Assumption:

\[ R(P_4) = \{ \text{Valve-\textit{air},i} \in [54.777, 69.898] \land \text{xInfuent,i} \in [28.792, 83.792] \land \text{xTemp-\textit{ww},i} \in [8.427, 13.327] \land \text{xTemp-\textit{ww},i} \in [3.327, 21.896] \} \]

Best Local concept and partial Close-World Assumption:

\[ R(P_4) = \{ \text{Valve-\textit{air},i} \in [54.777, 69.898] \land \text{xInfuent,i} \in [28.792, 83.792] \land \text{xTemp-\textit{ww},i} \in [8.427, 13.327] \land \text{xTemp-\textit{ww},i} \in [3.327, 21.896] \} \]
of BbD and an interactive combination of concepts upon hierarchical subdivisions of the domain. Benefits of this proposal are specially interesting in the interpretation of partitions with a large number of classes. Automatic generation of interpretations cover the important goal of KDD of describing the domain Fayyad and et al. [1996]. However, in this proposal a direct connection between the generated concepts and the automatic rules generation allows direct construction of a decision model for the later class prediction. As a matter of a fact, automatic production of probabilistic or fuzzy classification rules regarding concepts provided by CCEC is direct, as discussed in Gibert and Pérez-Bonilla [2005]. By associating an appropriate characteristic to every class, a model for operating the waste water treatment plant on a concrete day is obtained upon discussing in Gibert and Pérez-Bonilla [2005]. By associating an appropriate characteristic to every class, a model for operating the waste water treatment plant on a concrete day is obtained upon discussing in Gibert and Pérez-Bonilla [2005].

### Table 1: Comparison among the 5 proposals

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<th>(#(C))</th>
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<th>(#(R \cup C))</th>
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- **CCEC**: This method provides direct connections between generated concepts and the automatic rules generation, allowing direct construction of a decision model for the later class prediction.
- **BL**: A method that aims to provide results much more connected to the interpretation proposed by the expert than the results provided by CCEC.
- **CW A**: A method that provides solutions that may include class-redundant variables.
- **DR**: A method that guarantees the most compact concepts but may include class-redundant variables.
- **BbD**: An interactive combination of concepts upon hierarchical subdivisions of the domain.
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