

# Mr-SBC: a Multi-Relational Naïve Bayes Classifier

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**Abstract.** In this paper we propose an extension of the naïve Bayes classification method to the multi-relational setting. In this setting, training data are stored in several tables related by foreign key constraints and each example is represented by a set of related tuples rather than a single row as in the classical data mining setting. This work is characterized by three aspects. First, an integrated approach in the computation of the posterior probabilities for each class that make use of first order classification rules. Second, the applicability to both discrete and continuous attributes by means a supervised discretization. Third, the consideration of knowledge on the data model embedded in the database schema during the generation of classification rules. The proposed method has been implemented in the new system Mr-SBC, which is tightly integrated with a relational DBMS. Testing has been performed on two datasets and four benchmark tasks. Results on predictive accuracy and efficiency are in favour of Mr-SBC for the most complex tasks.

## 1 Introduction

Many inductive learning algorithms assume that the training set can be represented as a single table, where each row corresponds to an example and each column to a predictor variable or to the *target* variable  $Y$ . This assumption, also known as *single-table assumption* [23], seems quite restrictive in some data mining applications, where data are stored in a database and are organized into several tables for reasons of efficient storage and access. In this context, both predictor variables and the target variable are represented as attributes of distinct tables (relations).

Although in principle it is possible to consider a single relation reconstructed by performing a relational join operation on the tables, this approach is fraught with many difficulties in practice [2,11]. It produces an extremely large, and impractical to handle, table with lots of data being repeated. A different approach is the construction of a single central relation that summarizes and/or aggregates information which can be found in other tables. Also this approach has some drawbacks, since information about how data were originally structured is lost. Consequently, the (multi-)relational data mining approach has been receiving considerable attention in the literature, especially for the classification task [1,10,15,20,7].

In the traditional classification setting [18], data are generated independently and with an identical distribution from an unknown distribution  $P$  on some domain  $\mathbf{X}$  and are labelled according to an unknown function  $g$ . The domain of  $g$  is spanned by  $m$

independent (or predictor) random variables  $X_i$  (both numerical and categorical), that is  $\mathbf{X}=X_1 \times X_2 \times \dots \times X_m$ , while the range of  $g$  is a finite set  $Y=\{C_1, C_2, \dots, C_L\}$ , where each  $C_i$  is a distinct class. An inductive learning algorithm takes a training sample  $S=\{(\mathbf{x}, y) \in \mathbf{X} \times Y \mid y=g(\mathbf{x})\}$  as input and returns a function  $f$  which is hopefully close to  $g$  on the domain  $\mathbf{X}$ . A well-known solution is represented by the Naïve Bayesian Classifiers [3], which aim to classify any  $x \in \mathbf{X}$  is the class maximizing the *posterior probability*  $P(C_i|x)$  that the observation  $x$  is of class  $C_i$ , that is:

$$f(\mathbf{x}) = \arg \max_i P(C_i|x)$$

By applying the Bayes theorem,  $P(C_i|x)$  can be reformulated as follows:

$$P(C_i|x) = \frac{P(C_i)P(x|C_i)}{P(x)}$$

where the term  $P(x|C_i)$  is in turn estimated by means of the *naïve Bayes assumption*:

$$P(x|C_i) = P(x_1, x_2, \dots, x_m|C_i) = P(x_1|C_i) \times P(x_2|C_i) \times \dots \times P(x_m|C_i)$$

This assumption is clearly false if the predictor variables are statistically dependent. However, even in this case, the naïve Bayesian classifier can give good results [3].

In this paper we present a new approach to the problem of learning classifiers from relational data. In particular, we intend to extend the naïve Bayes classification to the case of relational data. Our proposal is based on the induction of a set of first-order classification rules in the context of naïve Bayesian classification.

Studies on first-order naïve Bayes classifiers have already been reported in the literature. In particular, Pompe and Kononenko [20] proposed a method based on a two-step process. The first step uses the ILP-R system [21] to learn a hypothesis in the form of a set of first-order rules and then, in the second step, the rules are probabilistically analyzed. During the classification phase, the conditional probability distributions of individual rules are combined naïvely according to the naïve Bayesian formula.

Flach and Lachiche proposed a similar two-step method, however, unlike the previous one, there is no learning of first-order rules in the first step. Alternatively, a set of patterns (first-order conditions) is generated that are used afterwards as attributes in a classical attribute-value naïve Bayesian classifier [7]. IBC, the system implementing this method, views individuals as structured objects and distinguishes between *structural* predicates referring to parts of individuals (e.g. atoms within molecules), and *properties* applying to the individual or one or several of its parts (e.g. a bond between two atoms). An *elementary first-order feature* consists of zero or more structural predicates and one property.

An evolution of IBC is represented by the system IBC2 [16], where no preliminary generation of first-order conditions is present. Predicates whose probabilities have to be estimated are dynamically defined on the basis of the individual to classify. Therefore, this is a form of *lazy* learning, which defers processing of its inputs (i.e., the estimation of the posterior probability according to the Bayesian statistical framework) until it receives requests for information (the class of the individual). Computed probabilities are discarded at the end of the classification process. Probability estimates are recursively computed and problems of non-termination in the computation may also occur.

An important aspect of the first two (*eager*) approaches is that they keep the phases of first-order rules/conditions generation and of probability estimation separate. In particular, Pompe and Kononenko use ILP-R to induce first-order rules [21], while IBC uses TERTIUS [8] to generate first order features. Then, the probabilities are computed for each first-order rule or feature. In the classification phase, the two approaches are similar to a multiple classifier because they combine the results of two algorithms. However, most first-order features or rules share some literals and this approach takes into account the related probabilities more than once. To overcome this problem it is necessary to rely on an integrated approach, so that the computation of probabilities on shared literals can be separated from the computation of probabilities on the remaining literals.

Systems implementing one of the three above approaches work on a set of main-memory Prolog facts. In real-world applications, where facts correspond to tuples stored on relational databases, some pre-processing is required in order to transform tuples into facts. However, this has some disadvantages. First, only part of the original hypothesis space implicitly defined by foreign key constraints can be represented after some pre-processing. Second, much of the pre-processing may be unnecessary, since a part of the hypothesis described by Prolog facts space may never be explored, perhaps because of early pruning. Third, in applications where data can frequently change, pre-processing has to be frequently repeated. Finally, database schemas provide the learning system free of charge with useful knowledge of data model that can help to guide the search process. This is an alternative to asking the users to specify a language bias, such as in IBC or IBC2.

A different approach has been proposed by Getoor [13] where the Statistical Relational Models (SRM) are learnt taking advance from the tightly integration with a database. SRMs are models very similar to Bayesian Networks. The main difference is that the input of a SRM learner is the relational schema of the database and the tuples of the tables in the relational schema.

In this paper the system Mr-SBC (Multi-Relational Structural Bayesian Classifier) is presented. It implements a new learning algorithm based on an integrated approach of first-order classification rules with naive Bayesian classification, in order to separate the computation of probabilities of shared literals from the computation of probabilities for the remaining literals. Moreover, Mr-SBC is tightly integrated with a relational database as in the work by Getoor, and handles categorical as well as numerical data through a discretization method.

The paper is organized as follows. In the next section the problem is introduced and defined. The induction of first-order classification rules is presented in Section 3, the discretization method is explained in Section 4 and the classification model is illustrated in Section 5. Finally, experimental results are reported in Section 6 and some conclusions are drawn.

## 2 Problem statement

In traditional classification systems that operate on a single relational table, an observation (or individual) is represented as a tuple of the relational table. Conversely, in Mr-SBC, which induces first-order classifiers from data stored in a set

$S=\{T_0, T_1, \dots, T_n\}$  of tables of a relational database, an individual is a tuple  $t$  of a *target* relation  $T$  joined with all the tuples in  $S$  which are related to  $t$  following a foreign key path. Formally, a foreign key path is defined as follows:

**Def 1.** A *foreign key path* is an ordered sequence of tables  $\vartheta=(T_{i_1}, T_{i_2}, \dots, T_{i_s})$ , where

- $\forall j=1, \dots, s, T_{i_j} \in S$
- $\forall j=1..s-1, T_{i_{j+1}}$  has a foreign key to the table  $T_{i_j}$

In Fig.1 an example of foreign key paths is reported. In this case,  $S=\{\text{MOLECULE}, \text{ATOM}, \text{BOND}\}$  and the foreign keys are:  $A\_M\_FK$ ,  $B\_M\_FK$ ,  $A\_A\_FK1$ ,  $A\_A\_FK2$ . If the target relation  $T$  is MOLECULE then five foreign key paths exists. They are: (MOLECULE), (MOLECULE,ATOM), (MOLECULE, BOND), (MOLECULE, ATOM, BOND) and (MOLECULE, ATOM, BOND). The last two are equal because the bond table has two foreign keys referencing the table atom.

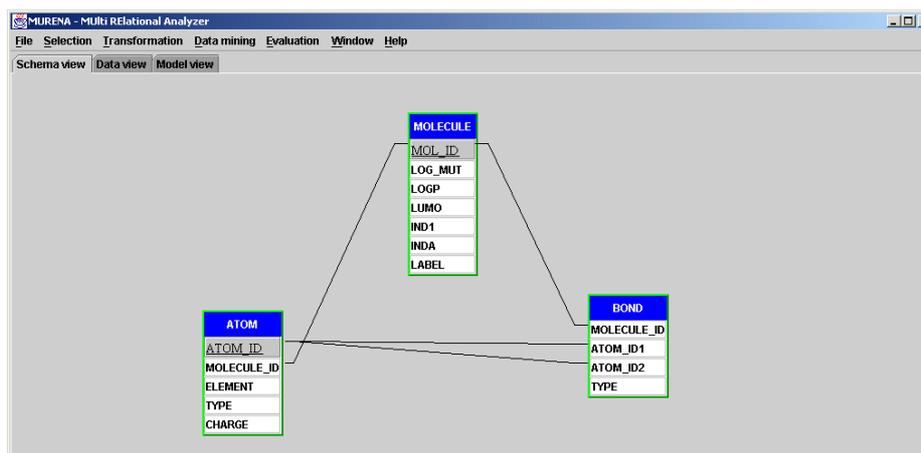
A formal definition of the learning problem solved by MR-SBC is the following problem:

*Given:*

- A *training set* represented by means of  $h$  relational tables  $S=\{T_0, T_1, \dots, T_n\}$  of a relational database  $D$ .
- A set of *primary key constraints* on tables in  $S$ .
- A set of *foreign key constraints* on tables in  $S$ .
- A *target relation*  $T(x_1, \dots, x_n) \in S$
- a *target discrete attribute*  $y$  in  $T$ , different from the primary key of  $T$ .

*Find:*

A naive Bayesian classifier which predicts the value of  $y$  for some individual represented as a tuple in  $T$  (with possibly UNKNOWN value for  $y$ ) and related tuples in  $S$  according to foreign key paths.



**Fig. 1.** An example of a relational representation of training data of the Mutagenesis database.

### 3 Generation of first-order rules

Let  $R'$  be a set of first-order classification rules for the classes  $\{C_1, C_2, \dots, C_L\}$ , and  $I$  an individual to be classified and defined as above. The individual can be logically represented as a set of ground facts, the only exception being the fact associated to the target relation  $T$ , where the argument corresponding to the target attribute  $y$  is a variable  $Y$ . A rule  $R_j \in R'$  covers  $I$ , if a substitution  $\theta$  exists, such that  $R_j\theta \subseteq I\theta$ . The application of the substitution to  $I$  is required to ground the only variable  $Y$  in  $I$  to the same constant as that reported in  $R_j$  for the target attribute. Let  $R$  be the subset of rules in  $R'$  that cover  $I$ , that is  $R = \{R_j \in R' \mid R_j \text{ covers } I\}$ . The first-order naïve Bayes classifier for the individual  $I$ ,  $f(I)$ , is defined as follows:

$$f(I) = \arg \max_i P(C_i|R) = \arg \max_i \frac{P(C_i)P(R|C_i)}{P(R)}$$

The value  $P(C_i)$  is the prior probability of the class  $C_i$ . Since  $P(R)$  is independent of the class  $C_i$ , it does not affect  $f(I)$ , that is,

$$f(I) = \arg \max_i P(C_i)P(R|C_i) \quad (1)$$

The computation of  $P(R|C_i)$  depends on the structure of  $R$ . Therefore, it is important to clarify how first-order rules are built in order to associate them with a probability measure. As already pointed out, Pompe and Kononenko use the first-order learning system ILP-R to induce the set of rules  $R'$ . This approach is very expensive and does not take into account the bias automatically determined by the constraints in the database. On the other hand, Flach and Lachiche use Tertius to determine the structure of *first-order features* on the basis of the structure of the individuals. The system Tertius deals with learning first-order logic rules from data lacking an explicit classification predicate. Consequently, the learned rules are not restricted to predicate definitions as in supervised inductive logic programming. Our solution is similar to that proposed by Flach since the structure of classification rules is determined on the basis of the structure of the individuals. The main difference is that the classification predicate is considered during the generation of the rules.

All predicates in classification rules generated by Mr-SBC are binary and can be of two different types.

**Def 2.** A binary predicate  $p$  is a *structural* predicate associated to a table  $T_i \in S$  if a foreign key  $FK$  in  $T_i$  exists that references a table  $T_{i'} \in S$ . The first argument of  $p$  represents the primary key of  $T_{i'}$  and the second argument represents the primary key of  $T_i$ .

**Def 3.** A binary predicate  $p$  is a *property* predicate associated to a table  $T_i \in S$ , if the first argument of  $p$  represents the primary key of  $T_i$  and the second argument represents another attribute in  $T_i$  which is neither the primary key of  $T_i$  nor a foreign key in  $T_i$ .

**Def 4.** A first order classification rule associated to the *foreign key path*  $\mathcal{G}$  is a clause in the form:

$$p_0(A_1, y) :- p_1(A_1, A_2), p_2(A_2, A_3), \dots, p_{s-1}(A_{s-1}, A_s), p_s(A_s, c).$$

where

1.  $p_0$  is a property predicate associated to the target table  $T$  and to the target attribute  $y$ .
2.  $\mathcal{Q}=(T_{i_1}, T_{i_2}, \dots, T_{i_s})$  is a *foreign key path* such that for each  $k=1, \dots, s-1$ :  $p_k$  is a structural predicate associated to the table  $T_{i_k}$
3.  $p_s$  is a property predicate associated to the table  $T_{i_s}$ .

An example of a first-order rule is the following:

*molecule\_Label(A, active) :- molecule\_Atom(A,B), atom\_Type(B, '[22..27]')*.

Mr-SBC searches all possible classification rules by means of a breadth-first strategy and iterates over some refining steps. A refining step is biased by the possible foreign key paths and consists of the addition of a new literal, the unification of two variables and, in the case of a property predicate, in the instantiation of a variable. The search strategy is biased by the structure of the database because each refining step is made only if the generated first-order classification rule can be associated to a foreign key path. However, the number of refinement steps is upper bounded by a user-defined constant `MAX_LEN_PATH`.

## 4 Discretization

In Mr-SBC continuous attributes are handled through supervised discretization. Supervised discretization methods utilize the information on the class labels of individuals to partition a numerical interval into bins. The proposed algorithm sorts the observed values of a continuous feature and attempts to greedily divide the domain of the continuous variable into bins, such that each bin contains only instances of one class. Since such a scheme could possibly lead to one bin for each observed real value, the algorithm is constrained to merge bins in a second step. Merging of two contiguous bins is performed when the increase of entropy is lower than a user-defined threshold (`MAX_GAIN`). This method is a variant of the one-step method IRD by Holte [14] for the induction of one-level decision trees, that proved to work well with the Naïve Bayes Classifier [4]. It is also different from the one-step method by Fayyad and Irani [6] that recursively splits the initial interval according to the class information entropy measure until a stopping criterion based on the Minimum Description Length (MDL) principle is verified.

## 5 The computation of probabilities

According to the naïve Bayes assumption, the attributes are considered independent. However, this assumption is clearly false for the attributes that are primary keys or foreign keys. This means that the computation of  $P(R|C_i)$  in equation (1) depends on the structures of rules in  $R$ . For instance, if  $R_1$  and  $R_2$  are two rules of class  $C_i$ , that share the same structure and differ only for the property predicates in their bodies

$$R_1: \beta_{1,0} : -\beta_{1,1}, \dots, \beta_{1,K_1-1}, \beta_{1,K_1}$$

$$R_2: \beta_{2,0} :- \beta_{2,1}, \dots, \beta_{2,K_2-1}, \beta_{2,K_2}$$

where

$$K_1=K_2 \text{ and } \beta_{1,1} = \beta_{2,1}, \beta_{1,2} = \beta_{2,2}, \dots, \beta_{1,K_1-1} = \beta_{2,K_2-1}$$

$$\text{then } P(\{R_1, R_2\} | C_i) = P(\beta_{1,0} \cap (\beta_{1,1}, \dots, \beta_{1,K_1-1}) \cap \beta_{1,K_1} \cap \beta_{2,K_2} | C_i) =$$

$$P(\beta_{1,0} \cap (\beta_{1,1}, \dots, \beta_{1,K_1-1}) | C_i) \cdot P(\beta_{1,K_1} \cap \beta_{2,K_2} | \beta_{1,0} \cap (\beta_{1,1}, \dots, \beta_{1,K_1-1}) \cap C_i)$$

The first term takes into account the structure common to both rules while the second term refers to the conditional probability of satisfying the property predicates in the rules given the common structure.

The latter probability can be factorized under the naïve Bayes assumption, that is:

$$P(\beta_{1,K_1} \cap \beta_{2,K_2} | \beta_{1,0} \cap (\beta_{1,1}, \dots, \beta_{1,K_1-1}) \cap C_i) =$$

$$P(\beta_{1,K_1} | \beta_{1,0} \cap (\beta_{1,1}, \dots, \beta_{1,K_1-1}) \cap C_i) \cdot P(\beta_{2,K_2} | \beta_{1,0} \cap (\beta_{1,1}, \dots, \beta_{1,K_1-1}) \cap C_i)$$

According to this approach the conditional probability of the structure is computed only once. This approach differs from that proposed in the works of Pompe and Kononenko [20] and Flach [7] where the factorization would multiply the structure probability twice.

By generalizing to a set of classification rules we have:

$$P(C_i)P(R | C_i) = P(C_i)P(\text{structure}) \prod_j P(R_j | \text{structure}) \quad (2)$$

where the term *structure* takes into account the class  $C_i$  and the structural parts of the rules in  $R$ .

If the classification rule  $R_j \in R$  is in the form  $\beta_{j,0} :- \beta_{j,1}, \dots, \beta_{j,K_j-1}, \beta_{j,K_j}$  where  $\beta_{j,0}$  and  $\beta_{j,K_j}$  are property predicates and  $\beta_{j,1}, \beta_{j,2}, \dots, \beta_{j,K_j-1}$  are structural predicates, then:

$$P(R_j | \text{structure}) = P(\beta_{j,K_j} | \beta_{j,0}, \beta_{j,1}, \dots, \beta_{j,K_j-1}) = P(\beta_{j,K_j} | C_i, \beta_{j,1}, \dots, \beta_{j,K_j-1})$$

where  $C_i$  is the value of the target attribute in the head of the clause ( $\beta_{j,0}$ ). To compute this probability, we use the Laplace estimation:

$$P(\beta_{j,K_j} | C_i, \beta_{j,1}, \dots, \beta_{j,K_j-1}) = \frac{\#(\beta_{j,K_j}, C_i, \beta_{j,1}, \dots, \beta_{j,K_j-1}) + 1}{\#(C_i, \beta_{j,1}, \dots, \beta_{j,K_j-1}) + F}$$

where  $F$  is the number of possible values of the attribute to which the  $\beta_{j,K_j}$  property predicate is associated. Laplace's estimate is used in order to avoid null probabilities in the equation (2). In practice, the value at the nominator is the number of individuals which satisfy that conjunction  $\beta_{j,K_j}, C_i, \beta_{j,1}, \dots, \beta_{j,K_j-1}$ , in other words, the number of individuals covered by the rule  $\beta_{j,0} :- \beta_{j,1}, \dots, \beta_{j,K_j-1}, \beta_{j,K_j}$ . It is determined by a "select count (\*)" SQL instruction. The value of the denominator is the number of individuals covered by the rule  $\beta_{j,0} :- \beta_{j,1}, \dots, \beta_{j,K_j-1}$ .

The term  $P(\text{structure})$  in the equation (2) is computed as follows: Let  $B = \{(\beta_{j,1}, \beta_{j,2}, \dots, \beta_{j,t}) | j=1..s \text{ and } t=1, \dots, K_j-1\}$  the set of all distinct sequences of structural predicates in the rules of  $R$ . Then

$$P(\text{structure}) = \prod_{\text{seq} \in B} P(\text{seq}) \quad (3)$$

To compute  $P(\text{seq})$  it is necessary to introduce the definition of the probability JP that a join query is satisfied, for this purpose, the formulation provided in [11] can be useful. Let  $\mathcal{Q} = (T_{i_1}, T_{i_2}, \dots, T_{i_s})$  be a *Foreign Key Path*, then:

$$JP(\mathcal{Q}) = JP(T_{i_1}, \dots, T_{i_s}) = \frac{|\triangleright \triangleleft (T_{i_1} \times \dots \times T_{i_s})|}{|T_{i_1}| \times \dots \times |T_{i_s}|}$$

where  $\triangleright \triangleleft (T_{i_1} \times \dots \times T_{i_s})$  is the result of the join between the tables  $T_{i_1}, \dots, T_{i_s}$ .

We must remember that each sequence  $\text{seq}$  is associated to a foreign key path  $\mathcal{Q}$ . If  $\text{seq} = (\beta_{j,1}, \beta_{j,2}, \dots, \beta_{j,t})$  there are two possibilities: either a prefix of  $\text{seq}$  is in  $B$  or not. By denoting as  $T_{j_h}$  the table related to  $\beta_{j,h}$ ,  $h=1, \dots, t$ , the probability  $P(\text{seq})$  can be recursively defined as follows:

$$P(\text{seq}) = \begin{cases} JP(T_{j_1}, \dots, T_{j_t}) & \text{if } \text{seq} \text{ has no prefix in } B \\ \frac{JP(T_{j_1}, \dots, T_{j_t})}{P(\text{seq}')} & \text{if } \text{seq}' \text{ is the longest prefix of } \text{seq} \text{ in } B \end{cases}$$

This formulation is necessary in order to compute the formula (3) considering both dependent and independent events. Since  $P(\text{structure})$  takes into account the class,  $P(\text{seq})$  is computed separately for each class.

## 6 Experimental Results

MR-SBC has been implemented as a module of the system MURENA and has been empirically evaluated on the Mutagenesis datasets and on Biodegradability datasets.

### 6.1 Results on Mutagenesis

These datasets, taken from the MLNET repository, concern the problem of identifying the mutagenic compounds [19] and have been extensively used to test both inductive logic programming (ILP) systems and (multi-)relational mining systems. We considered, analogously to related experiments in the literature, the ‘‘regression friendly’’ dataset of 188 elements.

A recent study on this database [22] recognizes five levels of background knowledge for mutagenesis which can provide richer descriptions of the examples. In this study we used only the first three levels of background knowledge in order to compare the performance of Mr-SBC with other methods for which experimental results are available in the literature. Table 1 shows the first three sets of background knowledge used in our experiments, where  $BK_i \subseteq BK_{i+1}$  for  $i=0, \dots, 2$ . The greater the BK, the more complex the learning problem.

**Table 1.** Background knowledge for Mutagenesis database.

Background	Description
$BK_0$	Consists of those data obtained with the molecular modelling package QUANTA. For each compound it obtains the atoms, bonds, bond types, atom types, and partial charges on atoms.
$BK_1$	Consists of Definitions in $B0$ plus indicators $ind1$ , and $inda$ in molecule table.
$BK_2$	Variables (attributes) $logp$ , and $lumo$ are added to definitions in $BK_1$ .

The dataset is analyzed by means of a 10-fold cross-validation, that is, the target table is first divided into ten blocks of near-equal size and distribution of class values, and then, for every block, a subset of tuples in  $S$  related to the tuples in the target table block are extracted. In this way, ten databases are created. Mr-SBC is trained on nine databases and tested on the hold-out database. Mr-SBC has been executed with the following parameters: MAX\_LEN\_PATH=4 and MAX\_GAIN= 0.5.

Experimental results on predictive accuracy are reported in Table 2 for increasing complexity of the models. A comparison to other results reported in the literature is also made. Mr-SBC has the best performance for the most complex task ( $BK_2$ ) with an accuracy of almost 90%, while it ranks third for the simplest task. Interestingly, the predictive accuracy increases with the complexity of the background knowledge, which means that the variables added in  $BK_1$  and  $BK_2$  are meaningful and Mr-SBC takes advantages of that.

As regards execution time (see Table 3). The time required by Mr-SBC increases with the complexity of the background knowledge. Mr-SBC is generally considerably faster than competing systems, such as Progol, Foil, Tilde and 1BC, that do not operate on data stored in a database. Moreover, except for the task  $BK_0$ , Mr-SBC performs better than MRDTL which works on a database. It is noteworthy that the trade-off between accuracy and complexity is in favour of Mr-SBC.

The average number of extracted rules for each fold is quite high (55.9 for  $BK_0$ , 59.9 for  $BK_1$ , and 64.8 for  $BK_2$ ). Some rules are either redundant or cover very few individuals. Therefore, some additional stopping criteria are required to avoid the generation of these rules and to reduce further the cost complexity of the algorithm.

**Table 2.** Accuracy comparison on the set of 188 regression friendly elements of Mutagenesis. Results for Progol2, Foil, Tilde are taken from [1]. Results for Progol\_1 are taken from [22]. The results for 1BC are taken from [9]. Results for 1BC2 are taken from [16]. Results for MRDTL are taken from [17]. The values are the results of 10-fold cross-validation.

System	Accuracy(%)		
	$BK_0$	$BK_1$	$BK_2$
Progol 1	79	86	86
Progol 2	76	81	86
Foil	61	61	83
Tilde	75	79	85
MRDTL	67	<b>87</b>	88
1BC2	72.9	---	72.9
1BC	<b>80.3</b>	---	87.2
Mr-SBC	76.5	81	<b>89.9</b>

**Table 3.** Time comparison of the set of 188 regression friendly elements of Mutagenesis. Results for Progol2, Foil, Tilde are taken from [1]. Results for Progol\_1 are taken from [22]. Results for MRDTL are taken from [17]. The results of MR-SBC have been taken on a PIII WIN2k platform.

System	Time (Secs)		
	$BK_0$	$BK_1$	$BK_2$
Progol 1	8695	4627	4974
Progol 2	117000	64000	42000
Foil	4950	9138	0.5
Tilde	41	170	142
MRDTL	0.85	170	142
1BC2	--	--	--
1BC	--	--	--
MR-SBC	36	42	48

## 6.2 Results on Biodegradability

The Biodegradability dataset has already been used in the literature for both regression and classification tasks [5]. It consists of 328 structural chemical molecules described in terms of atom and bond. The target variable for machine learning systems is the natural logarithm of the arithmetic mean of the low and high estimate of the HTL (Half-Life Time) for aqueous biodegradation in aerobic conditions, measured in hours. We use a discretized version in order to apply classification systems to the problem. As in [5], four classes have been defined: chemicals degrade *fast*, *moderately*, *slowly* or are *resistant*.

The dataset is analyzed by means of a 10-fold cross-validation. For each database Mr-SBC and Tilde are trained on nine databases and tested on the hold-out database. Mr-SBC has been executed with the following parameters: MAX\_LEN\_PATH=4 and MAX\_GAIN= 0.5. Experimental results on predictive accuracy are reported in Table 4. They are in favour of Mr-SBC on the average of accuracy varying the fold.

**Table 4.** Accuracy comparison on the set of 328 chemical molecules of Biodegradability. Results for Mr-SBC and Tilde are reported.

Fold	Mr-SBC	Tilde Pruned
0	<b>0.90909</b>	0.69697
1	<b>0.87878</b>	0.81818
2	0.84848	<b>0.90909</b>
3	0.87878	0.87879
4	<b>0.78788</b>	0.69697
5	0.84848	<b>0.90909</b>
6	0.90625	0.90625
7	<b>0.87879</b>	0.81818
8	0.87500	<b>0.93750</b>
9	<b>0.93939</b>	0.72727
Average	<b>0.87509</b>	0.82983

## 7 Conclusions

In the paper, a multi-relational data mining system with a tight integration to a relational DBMS is described. It is based on the induction of a set of first-order classification rules in the context of naive Bayesian classification. It presents several differences with respect to related works. First, it is based on an integrated approach, so that the contribution of literals shared by several rules to the posterior probability is computed only once. Second, it works both on discrete and continuous attributes. Third, the generation of rules is based on the knowledge of a data model embedded in the database schema. The proposed method has been implemented in the new system Mr-SBC and tested on four benchmark tasks. Results on predictive accuracy are in favour of our system for the most complex tasks. Mr-SBC also proved to be efficient.

As future work, we plan to extend the comparison of Mr-SBC to other multi-relational data mining systems on a larger set of benchmark datasets. Moreover, we intend to frame the proposed method in a transduction inference setting, where both labelled and unlabelled data are available for training. Finally we intend to integrate Mr-SBC in a document processing system that makes extensive use of machine learning tools to reach a high adaptivity to different tasks.

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## References

- [1] Blockeel, H. Top-down induction of first order logical decision trees. PhD dissertation, Department of Computer Science, Katholieke Universiteit Leuven, 1998.
- [2] De Raedt, L. Attribute-value learning versus Inductive Logic Programming: the Missing Links (Extended Abstract). In *Proceedings of the 8 th International Conference on Inductive Logic Programming*, volume 1446 of *Lecture Notes in Artificial Intelligence*, Springer-Verlag, 1998.
- [3] Domingos, P. & Pazzani, M.. On the optimality of the simple bayesian classifier under zero-one loss. *Machine Learning*, 29(2-3), pp. 103-130, 1997.
- [4] Dougherty, J., Kohavi, R., Sahami, M.: *Supervised and unsupervised discretization of continuous features*. In: Machine Learning: Proc of 12th International Conference. Morgan Kaufmann, pp.194-202. 1995.
- [5] Dzeroski S., Blockeel H., Kramer S., Kompare B., Pfahringer B., and Van Laer W.. Experiments in predicting biodegradability. *Proceedings of the Ninth International Workshop on Inductive Logic Programming* (S. Dzeroski and P. Flach, eds.), LNAI, vol. 1634, Springer, pp. 80-91, 1999.

- [6] Fayyad U.M., Irani K.B., Multi-interval discretization of continuous-valued attributes for classification learning. In Proc. Of the 13<sup>th</sup> International Joint Conference on Artificial Intelligence. pp.1022—1027, 1994.
- [7] Flach P.A. and Lachiche N.. Decomposing probability distributions on structured individuals. In Paula Brito, Joaquim Costa, and Donato Malerba, editors, *Proceedings of the ECML2000 workshop on Dealing with Structured Data in Machine Learning and Statistics*, pages 33--43, Barcelona, Spain, May 2000.
- [8] Flach P.A. and Lachiche N.. *Confirmation-guided discovery of first-order rules with Tertius*. Machine Learning, 2000.
- [9] Flach P. and Lachiche N.. First-order Bayesian Classification with 1BC. Submitted. Downloadable from <http://hydria.u-strasbg.fr/~lachiche/1BC.ps.gz>
- [10] Friedman, N., Getoor, L., Koller, D., and Pfeffer, A. Learning probabilistic relational models. In *Proceedings of the 6 th International Joint Conference on Artificial Intelligence*, Morgan Kaufman, 1999.
- [11] Getoor, L. Multi-relational data mining using probabilistic relational models: research summary. In: A. J. Knobbe, and D. M. G. van der Wallen, editors. *Proceedings of the First Workshop in Multi-relational Data Mining*, 2001.
- [12] Getoor L., Koller D., Taskar B. Statistical models for relational data. In Proceedings of the KDD-2002 Workshop on Multi-Relational Data Mining, pages 36-55, Edmonton, CA, 2002.
- [13] Getoor L.. Learning Statistical Models from Relational Data, Ph.D. Thesis, Stanford University, December, 2001.
- [14] Holte, R.C. Very simple classification rules perform well on most commonly used datasets, *Machine Learning* 11, pp. 63-90, 1993.
- [15] Krogel, M., and Wrobel, S. Transformation-Based Learning Using Multirelational Aggregation. In Céline Rouveirol and Michèle Sebag, editors, *Proceedings of the 11 th International Conference on Inductive Logic Programming*, vol. 2157 of *Lecture Notes in Artificial Intelligence*, Springer-Verlag, 2001.
- [16] Lachiche N. and Flach P.. 1BC2: a true first-order Bayesian classifier. In Claude Sammut and Stan Matwin, ed., *Proceedings of the Thirteenth International Workshop on Inductive Logic Programming (ILP'02)*, Sydney, Australia. LNAI 2583, Springer. pp. 133-148. 2003.
- [17] Leiva H.A.:MRDTL: *A multi-relational decision tree learning algorithm*. Master thesis, University of Iowa, USA, 2002.
- [18] Mitchell, T. *Machine Learning*. McGraw Hill, 1997.
- [19] Muggleton S. H., Bain M., Hayes-Michie J., Michie D.. An experimental comparison of human and machine learning formalisms. In Proc. Sixth International Workshop on Machine Learning, Morgan Kaufmann, San Mateo, CA, pp. 113--118, 1989.
- [20] Pompe U. and Kononenko I.. Naive Bayesian classifier within ILP-R. In L. De Raedt, editor, *Proc. of the 5th Int. Workshop on Inductive Logic Programming*, pages 417--436. Dept. of Computer Science, Katholieke Universiteit Leuven, 1995.
- [21] Pompe U., Kononenko I.. Linear space induction in first order logic with relief. In R. Kruse, R. Viertl. & G. Della Riccia (Eds.), *CISM Lecture Notes*. Udine Italy, 1994.
- [22] Srinivasan, A., King, R. D., and Muggleton, S. The role of background knowledge: using a problem from chemistry to examine the performance of an ILP program. Technical Report PRG-TR-08-99, Oxford University ComputingLaboratory, Oxford, 1999.
- [23] Wrobel, S. Inductive logic programming for knowledge discovery in databases. In: Džeroski, S., N. Lavrač(eds.): *Relational Data Mining*, Springer: Berlin, pp. 74-101. 2001.